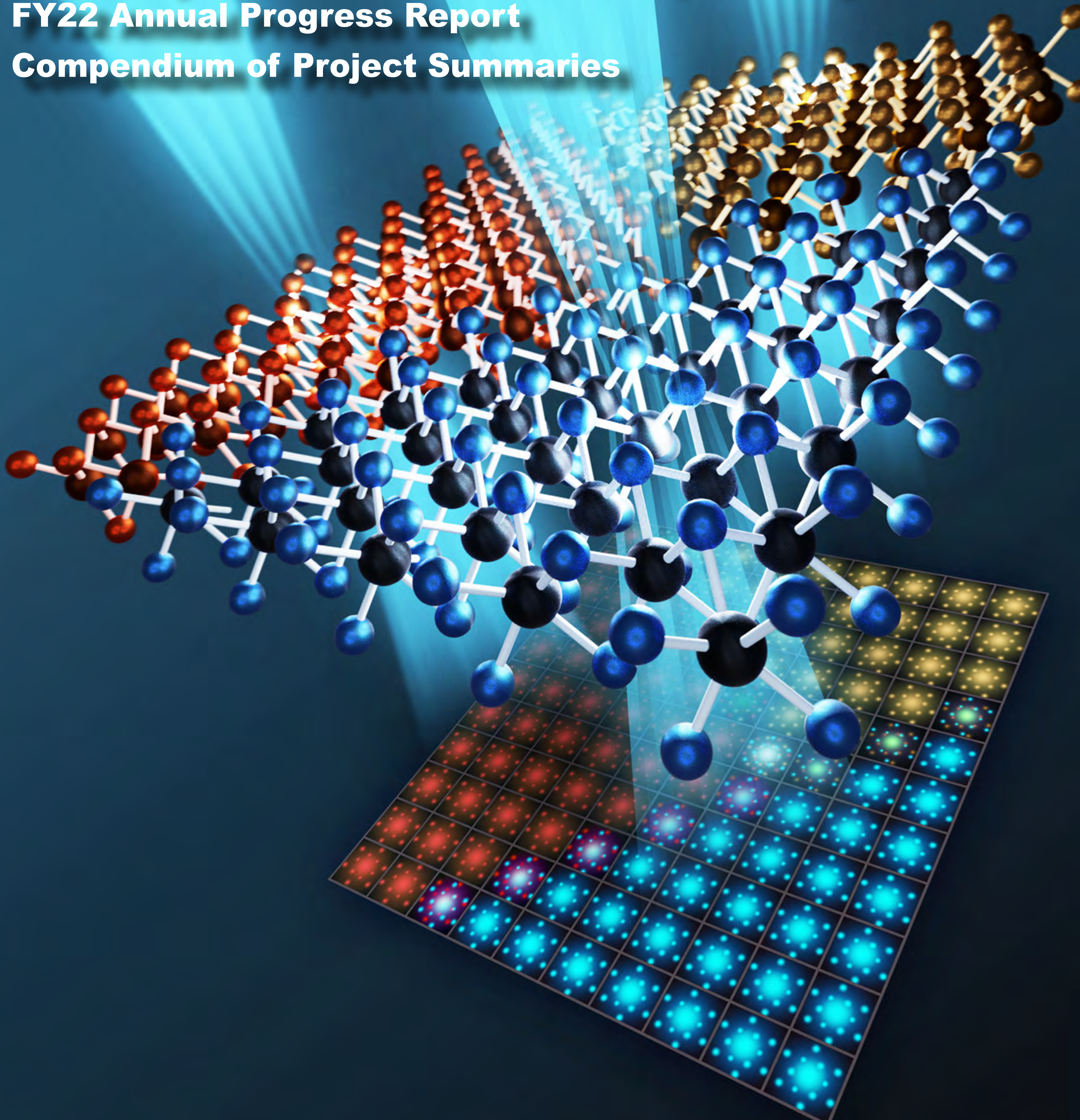
Los Alamos National Laboratory

Laboratory Directed Research and Development Program

FY22 Annual Progress Report

Compendium of Project Summaries



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LDRD
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LABORATORY DIRECTED RESEARCH & DEVELOPMENT

WHERE INNOVATION BEGINS

FY22 Annual Report

Compendium of Project Summaries

The project summaries are organized by Capability Pillar – Complex Natural and Engineered Systems, Information Science and Technology, Materials for the Future, Nuclear and Particle Futures, Science of Signatures, and Weapons Systems. Project summaries for continuing projects appear first, followed by project summaries and technical outcomes for projects that ended in FY22.

All images included with the project summaries are credited to Los Alamos National Laboratory unless otherwise noted.

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The Annual Report is available at:
https://www.lanl.gov/projects/ldrd-tri-lab/annual-reports.php.

On the Cover
Cover Image: This image shows the overall concept of a capability developed in LDRD project 202204856MFR led by Michael Pettes. Image shows a four-dimensional scanning transmisison electron microscopy. Artwork by Sarah Tasseff of Los Alamos National Laboratory

On the Inside Cover
National Security Sciences Building, Los Alamos National Laboratory. Photo credit: LANL

LA-UR-23-23288

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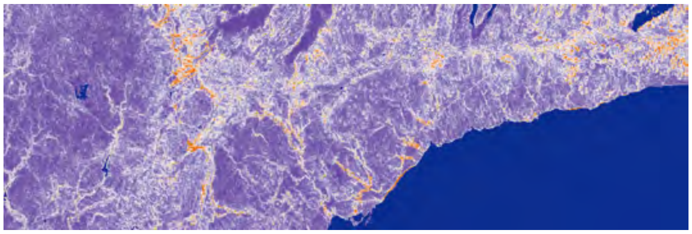
Complex Natural and Engineered Systems

Model-Driven Data Fusion for Disease Forecasting

Carrie Manore
20210062DR



Accurately predicting the how climate will impact mosquito-borne diseases and how we can best mitigate them requires new models that integrate climate, mosquito population, human demography/ infrastructure and disease transmission models. The Climate Integrated Model of Mosquito-borne Infectious Diseases, built with LDRD support, is capable of the model-data fusion at the continental scale needed to forecast future risk under various climate and human response scenarios. The model and its scaling and data-fusion capabilities can be used for multiple human-natural systems to provide decision makers with validated predictions.

Project Description

As humans travel more frequently and global change accelerates, global systems become increasingly stressed, leading to large-scale infectious disease outbreaks. Zika and chikungunya viruses spread across North and South America in a matter of months and coronavirus (COVID-19) went from a regional concern to a pandemic in less than two months. Vector-borne diseases in North America have increased 300% since between 2004-2016. Preparedness in this context means being able to run “what-if” scenarios. The data available and the computational tools have now advanced enough that we can predict future vector-borne diseases with a changing environment. Our model will be the first ever process-based mosquito-borne disease model that integrates all of the critical processes of hydrology, vegetation, mosquito, human, and disease transmission via Earth Systems Models for forecasting and "what-if" planning scenarios at the continental scale. Global security risks arising from infectious disease spread can only be anticipated through the integration of a multi-domain approach that combines mechanistic modeling with highly heterogeneous, multi-scale datasets that represent evolving systems.

Publications

Journal Articles

K. Albrecht, L. M. and K. A. Kaufeld. Investigating the impact of environmental factors on West Nile virus cases in Ontario, Canada. Submitted to *Frontiers in Public Health*. (LA-UR-22-32109)

*Castro, L. A., N. Generous, W. Luo, A. Pastore y Piontti, K. Martinez, M. F. C. Gomes, D. Osthus, G. Fairchild, A. Ziemann, A. Vespignani, M. Santillana, C. A. Manore and S. Y. Del Valle. Using heterogeneous data to identify signatures of dengue outbreaks at fine spatio-temporal scales across Brazil. 2021. *PLOS Neglected Tropical Diseases*. **15** (5): e0009392. (LA-UR-20-29637 DOI: 10.1371/journal.pntd.0009392)

*Cuellar, L., I. Torres, E. Romero-Severson, R. Mahesh, N. R. Ortega, S. A. Pungitore, N. W. Hengartner and R. Ke. Excess deaths reveal the true spatial, temporal and demographic impact of COVID-19 on mortality in Ecuador. 2021. *International Journal of Epidemiology*. (LA-UR-21-21361 DOI: 10.1093/ije/dyab163)

Fair, J. M., C. A. Manore and C. Xu. How will vector borne diseases change in the future with a changing climate?. Submitted to *GovOpenAccess Science Updates*. (LA-UR-21-29386)

. B. A. W. *. T. S. D. *. R. D. *. S. D. P. *. F. J. M. *. K. K. A. *. D. V. S. Y. *. M. C. A. Gorris, M. E., M. E. Gorris, A. W. Bartlow, S. D. Temple, J. M. Fair, K. A. Kaufeld, S. Y. Del Valle, C. A. Manore, D. Romero-Alvarez and D. P. Shutt. Updated distribution maps of predominant Culex mosquitoes across the Americas. 2021. *Parasites & Vectors*. **14 (1): 547. (LA-UR-21-24460 DOI: 10.1186/s13071-021-05051-3)

*Gorris, M. E., A. W. Bartlow, S. D. Temple, D. Romero-Alvarez, D. P. Shutt, J. M. Fair, K. A. Kaufeld, S. Y. Del Valle and C. A. Manore. Updated distribution maps of predominant Culex mosquitoes across the Americas. 2021. *Parasites & Vectors*. **14** (1): 547. (LA-UR-21-24422 DOI: 10.1186/s13071-021-05051-3)

Gorris, M. E., J. T. Randerson, S. R. Coffield, K. K. Treseder, C. S. Zender, C. Xu and C. A. Manore. Climate controls on the spatial pattern of West Nile virus incidence in the United States. Submitted to *Environmental Health Perspectives*. (LA-UR-22-20129)

Hapairi, L., K. Mysore, L. James, N. Scheel, J. Realey, L. Gerber, R. Shui Feng, E. Romero-Severson, A. Mohammed, M. Duman-Scheel and D. Severson. Evaluation of large volume yeast interfering RNA lure-and-kill ovitraps for attraction and control of Aedes mosquitoes. Submitted to *Medical and Veterinary Entomology*. (LA-UR-20-29552)

*Hepler, S. A., K. A. Kaufeld, K. Benedict, M. Toda, B. R. Jackson, X. Liu and D. Kline. Integrating Public Health Surveillance and Environmental Data to Model Presence of Histoplasma in the United States. 2022. *Epidemiology*. **33** (5): 654-659. (LA-UR-21-26964 DOI: 10.1097/EDE.0000000000001499)

Holcomb, K. M., M. A. Johansson, S. Mathis, C. M. Baker, J. E. Staples, M. Fischer, R. J. Nett, C. B. Beard, E. A. Mordecai, M. L. Childs, D. Kirk, M. J. Harris, N. Nova, M. P. Kain, A. C. Keyel, I. Rochlin, M. Marcantonio, E. L. Ray, J. M. Humphreys, L. W. Cohnsteadt, B. D. Hollingsworth, E. M. Reed, A. S. Freedman, M. Hamins-Puertolas, P. Das and M. E. Gorris. Evaluation of an open forecasting challenge to assess skill of West Nile virus neuroinvasive disease prediction. Submitted to *Parasites and Vectors*. (LA-UR-22-26001)

Trejo Lorenzo, I., M. J. Barnard, J. A. Spencer, J. Keithley, K. M. Martinez, I. K. Crooker, N. W. Hengartner, E. Romero-Severson and C. A. Manore. Changing temperature profiles and the risk of dengue outbreaks. Submitted to *PLOS Climate*. (LA-UR-22-20436)

Mancuso, M. L., C. A. Manore, K. M. Martinez and F. Milner. Numerical Issues for a Non-autonomous Logistic Model. Submitted to *Applied Mathematics Letters*. (LA-UR-22-27036)

Mancuso, M. L., K. M. Martinez, C. A. Manore, M. J. Barnard, F. Milner and H. C. Godinez Vazquez. Fusing time-varying mosquito data and continuous mosquito population dynamics models. Submitted to *Frontiers in Applied Mathematics and Statistics*. (LA-UR-23-23285)

Manore, C. A., D. A. Romero-Alvarez, L. Escobar, A. Auguste and S. Y. Del Valle. Transmission Risk of Oropouche Fever in the Americas. Submitted to *PNAS*. (LA-UR-22-25926)

Martinez, K. M., S. Pankavich, A. S. Siraj, G. Fairchild, A. Ziemann, S. Y. Del Valle and C. A. Manore. An unsupervised multi-objective feature selection method with applications to environmental and demographic data in Brazil. Submitted to *SIAM Journal on Mathematics of Data Science*. (LA-UR-22-20064)

Moser, S. K., M. J. Barnard, R. M. Frantz, J. A. Spencer, K. A. Rodarte, I. K. Crooker, A. W. Bartlow, E. Romero-Severson and C. A. Manore. Review of temperature-dependent life history traits of four Culex mosquito species (Diptera: Culicidae) and applications in disease modeling. Submitted to *PLOS Neglected Tropical Diseases*. (LA-UR-22-28538)

Moser, S., M. J. Barnard, R. M. Frantz, J. A. Spencer, K. A. Rodarte, I. K. Crooker, A. W. Bartlow, E. Romero-Severson and C. A. Manore. Scoping review of Culex mosquito life history trait heterogeneity in response to temperature. Submitted to *Parasites & Vectors*. (LA-UR-23-20412)

*Spencer, J. A., D. P. Shutt, S. K. Moser, H. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Distinguishing viruses responsible for influenza-like illness. 2022. *Journal of Theoretical Biology*. **545**: 111145. (LA-UR-21-27457 DOI: 10.1016/j.jtbi.2022.111145)

Spencer, J. A., D. P. Shutt, S. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Description of ILI General

Model Code. Submitted to *Journal of Theoretical Biology*. (LA-UR-22-24722)

Spencer, J. A. and K. M. Skogstad. Changing Temperatures, Changing Risks. Submitted to *SIAM News Online*. (LA-UR-23-21645)

*Temple, S. D., C. A. Manore and K. A. Kaufeld. Bayesian time-varying occupancy model for West Nile virus in Ontario, Canada. 2022. *Stochastic Environmental Research and Risk Assessment*. **36** (8): 2337-2352. (LA-UR-21-31764 DOI: 10.1007/s00477-022-02257-4)

Conference Papers

DeMets, S. A., A. Ziemann, C. Russell and C. A. Manore. Improving mosquito population models over the Greater Toronto Area using MSI and SAR data. Presented at *SPIE Defense and Commercial Sensing*. (Kissimmee, Florida, United States, 2021-04-12 - 2021-04-16). (LA-UR-21-23771)

Reports

Molina-Paris, C., G. Lythe, M. Lopez-Garcia, M. Locke, T. Finnie, T. Tipton and M. Carroll. Ebola Virus Inhibition of Type I Interferons. Unpublished report. (LA-UR-21-21631)

Presentation Slides

K. Albrecht, L. M. and K. A. Kaufeld. A Spatio-temporal Model to estimate West Nile virus cases in Ontario, CA. Presented at *SIAM Annual Meeting*, Pittsburgh, Pennsylvania, United States, 2022-07-11 - 2022-07-16. (LA-UR-22-26758)

DeMets, S. A., A. Ziemann, C. Russell and C. A. Manore. Improving mosquito population models over the Greater Toronto Area using MSI and SAR data. Presented at *SPIE Defense and Commercial Sensing*, Kissimmee, Florida, United States, 2021-04-12 - 2021-04-16. (LA-UR-21-23369)

Fair, J. M. Emerging Zoonotic Pathogens, Global Cooperative Threat Reduction & Scientific Collaboration. Presented at *Seminar University of New Mexico*, LOS ALAMOS, New Mexico, United States, 2021-04-19 - 2021-04-19. (LA-UR-21-23625)

Fair, J. M. and C. A. Manore. Vector Borne Disease Surveillance. Presented at *DOE National Lab Capabilities Managing Climate-Drive Zoontoc Disease Risk*, Washington, District Of Columbia, United States, 2022-07-20 - 2022-07-21. (LA-UR-22-27320)

Gorris, M. E. Life at LANL as an Earth System Scientist, and the new field of GeoHealth. . (LA-UR-22-25545)

Gorris, M. E., C. A. Manore and R. A. Hodge. The Shifting Distribution of Aedes Mosquitoes in Response to Changing Geographic Factors. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27624)

Hodge, R. A. The Shifting Distribution of Aedes Mosquitoes in Response to Changing Geographic Factors. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27701)

Kaufeld, K. A. Mosquitoes everywhere! Modeling Vector Borne Diseases in a Changing Environment. Presented at *SAMSI student workshop*, Virtual, New Mexico, United States, 2021-07-14 - 2021-07-14. (LA-UR-21-26709)

Kaufeld, K. A. Model-Driven Data Fusion for Infectious Disease in a Changing Environment. Presented at *Joint Statistical Meetings*, Virtual, New Mexico, United States, 2021-08-11 - 2021-08-11. (LA-UR-21-28014)

Kaufeld, K. A. and L. M. K. Albrecht. A Spatio-temporal Model to estimate West Nile virus cases in Ontario, CA. . (LA-UR-21-29672)

Trejo Lorenzo, I., M. J. Barnard, J. A. Spencer, J. S. Keithley, K. M. Martinez, I. K. Crooker, N. W. Hengartner, E. Romero-Severson and C. A. Manore. Assessing the Risk of Dengue Outbreaks in Three U.S. Cities. Presented at *Innovations in Climate Resilience (Battelle/DOE)*, Columbus, Ohio, United States, 2022-03-29 - 2022-03-30. (LA-UR-22-22257)

Mancuso, M. L. Climate and infection-age on West Nile Virus transmission. . (LA-UR-22-31113)

Manore, C. A. Model Driven Data Fusion for Disease Forecasting. Presented at *BIRS Pandemic Preparedness*, Kelowna, Canada, 2022-06-13 - 2022-06-17. (LA-UR-22-25925)

Manore, C. A. Climate-Driven Model for Mosquito-borne Disease. Presented at *ICMA VIII*, Lafayette, Louisiana, United States, 2022-10-28 - 2022-10-30. (LA-UR-22-31651)

Manore, C. A., M. K. Owusu and K. A. Kaufeld. EBird Sampling to Model West Nile Virus. Presented at *South Texas One Health Symposium*, Brownsville, Texas, United States, 2022-10-06 - 2022-10-06. (LA-UR-22-30790)

Martinez, K. M., C. A. Manore, S. Y. Del Valle, G. Fairchild, A. Ziemann, N. K. Parikh, L. A. Castro, K. C. Kempfert, D. A. Romero-Alvarez and E. N. A. Generous. Data Fusion and Disease Forecasting for Dengue in Brazil. . (LA-UR-21-31403)

Martinez, K. M. and D. A. Florez Pineda. Estimating the Mosquito Population Density in North America. Presented at *T Division Student Lightning Talks*, LOS ALAMOS, New Mexico, United States, 2022-08-09 - 2022-08-09. (LA-UR-22-28222)

Martinez, K. M. and M. L. Mancuso. Time-varying processes and infection-age on West Nile Virus transmission. Presented at *Workshop on Climate Change, Human Behavior, and Vector-bourne Disease Transmission*, Davis, California, United States, 2022-05-19 - 2022-05-20. (LA-UR-22-24598)

Moser, S. K., A. W. Bartlow and C. A. Manore. Culex spp. Mosquito Life History Traits and Applications in Disease Modeling. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-07-29 - 2022-07-29. (LA-UR-22-27716)

Spencer, J. A. Distinguishing viruses responsible for ILI to motivate increased viral surveillance. Presented at *BIRS Preparing for the Next Pandemic*, Kelowna, Canada, 2022-06-12 - 2022-06-17. (LA-UR-22-25538)

Spencer, J. A. Temperature Dependence in Dengue and West Nile Virus: Leveraging Mathematical Biology to Enhance National and Global Health Security. Presented at *8th Annual Intelligence Community Academic Research Symposium (ICARS) 2022*, Virtual, District Of Columbia, United States, 2022-09-21 - 2022-09-21. (LA-UR-22-29750)

Spencer, J. A., D. P. Shutt, S. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. What is Influenza-Like Illness?. Presented at *University of Florida Biomath Seminar*, Virtual, Florida, United States, 2022-02-10 - 2022-02-10. (LA-UR-22-21913)

Spencer, J. A., M. J. Barnard, C. A. Manore, E. J. Scully and A. Nguy-Robertson. Mapping Forecasting Error for Dengue in Brazil at High Resolution. Presented at *AmeriGEO Week 2021*, Washington, District Of Columbia, United States, 2021-08-23 - 2021-08-27. (LA-UR-21-28447)

Spencer, J. A., M. J. Barnard, I. Trejo Lorenzo, J. S. Keithley, K. M. Martinez, I. K. Crooker, N. W. Hengartner, E. Romero-Severson and C. A. Manore. Changing Temperatures and the Risk of Dengue Outbreaks. Presented at *SIAM Annual Meeting*, Virtual, New Mexico, United States, 2022-07-13 - 2022-07-15. (LA-UR-22-26778)

Spencer, J. A., M. J. Barnard, K. M. Martinez, A. R. Daughton, C. A. Manore, E. J. Scully and A. Nguy-Robertson. Searching Social Media for Signs of Dengue in Brazil. Presented at *American Geophysical Union Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31857)

Spencer, J. A., M. J. Barnard, K. M. Martinez, N. K. Parikh and C. A. Manore. Using Social Media to Improve Dengue Nowcasting in Brazil. Presented at *GEO Health Community of Practice Meeting*, Virtual, New Mexico, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32280)

Del Valle, S. Y. and L. A. Castro. Using Social Media & News Media for Real World Events. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-07. (LA-UR-23-22318)

Godinez Vazquez, H. C., D. A. Shutt, K. M. Martinez and C. A. Manore. Data Assimilation for a Process-Based Mosquito Density Model: Parameter Estimation using Ensemble Kalman Filter. Presented at *AGU Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31963)

Posters

K. Albrecht, L. M. and K. A. Kaufeld. Spatio-Temporal Model of West Nile Virus in Ontario, CA. Presented at *ENVR 2022 Workshop: Environmental and Ecological Research with Societal Impacts*, Provo, Utah, United States, 2022-10-06 - 2022-10-08. (LA-UR-22-30362)

Gorris, M. E., M. J. Barnard, S. Moser, J. A. Spencer, J. M. Hyman and C. A. Manore. Forecasting West Nile Virus in the United States Using Regional Disease Incidence and Climate Variability. Presented at *2022 CSTE/CDC Infectious Disease Forecasting Workshop*, Atlanta, Georgia, United States, 2022-10-25 - 2022-10-25. (LA-UR-22-31254)

Kaufeld, K. A., S. Moser and C. A. Manore. Data-Driven Bird Population Models using Statistical and Dynamical Surrogate Model Methods. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-33022)

Manore, C. A. and R. M. Frantz. Summer 2021 Los Alamos National Lab Internship. Presented at *Science Policy Management Exchange*, Logan, Utah, United States, 2021-09-24 - 2021-09-24. (LA-UR-21-29045)

Martinez, K. M., M. L. Mancuso, C. A. Manore and F. Milner. Climate and Infection-age on West Nile Virus Transmission. Presented at *ARCS Scholar Awards Dinner*, Phoenix, Arizona, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-23005)

Moser, S., J. A. Spencer, M. J. Barnard, J. M. Hyman, C. A. Manore and M. E. Gorris. Think Outside the Map: Using Ecoregions for Enhanced Disease Forecasting. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-07. (LA-UR-23-22387)

Moser, S., M. J. Barnard, R. M. Frantz, J. A. Spencer, K. A. Rodarte, I. K. Crooker, A. W. Bartlow, E. Romero-Severson and C. A. Manore. Temperature-Dependent Life History Traits in Culex Mosquito Disease Vectors. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-12. (LA-UR-22-32836)

Florez Pineda, D. A., E. Romero-Severson, S. Eshun, C. Franco, J. S. Keithley, M. L. Mancuso, J. A. Spencer, K. M. Martinez and C. A. Manore. Assessing the Risk of Dengue Outbreaks across Continental Biomes in Brazil. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27643)

Rodriguez-Chavez, D., M. E. Gorris and A. W. Bartlow. Assessing the Correlation Between Spring Bird Migrations and West Nile Virus. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27746)

Other

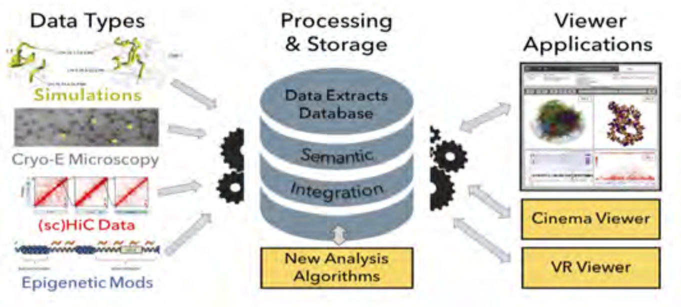
Fairchild, G., N. K. Parikh, J. P. Schwenk, J. S. Keithley and C. Xu. CIMMID Architecture Team Presents: How I Learned to Stop Worrying and Love Git/GitLab. Audio/Visual. (LA-UR-21-22181)

Gorris, M. E., A. W. Bartlow, S. D. Temple, D. A. Romero-Alvarez, D. A. Shutt, J. M. Fair, K. A. Kaufeld, S. Y. Del Valle and C. A. Manore. netCDF files of Culex habitat suitability values. Dataset. (LA-UR-21-24576)

**Peer-reviewed*

A 4-Dimensional Human Genome Project: Accelerating the Next Generation of Biological Discovery

Shawn Starkenburg
20210082DR



The existing linear, one dimensional human genome map is not sufficient to fully understand how cells function. In this project, we are developing an analysis platform that allows biologists for the first time to calculate and view time-dependent 3D models of chromosomes. These modifications will be visualized in a novel web-based tool that will quickly generate 4D genome maps. Knowledge revealed through this work will uncover the relevant genome locations that can be targets for treatment and may uncover unique patterns and signatures that in theory, can discriminate and diagnose exposure to chemical, biological, radiological, or nuclear events.

Project Description

Mapping the human genome transformed the face of science. However, this original linear, one dimensional genome map is not sufficient to fully understand how cells function. The same genome sequence can have dramatically different three dimensional (3D) structures that change over time (4-Dimensional) to control the function of our DNA. These dynamic structural changes underpin all biological functions. Thus, characterizing fundamental, healthy genome architectures (and virus or other pathogen-induced alterations) can expand strategies that counter biological, chemical, and radiological threats. In this project, we will develop an analysis platform that allows biologists for the first time to calculate and view time-dependent 3D models of chromosomes corresponding to specific stages of development or environmental conditions. These modifications will be visualized in a novel web-based tool that will quickly generate 4D genome maps based on experimental data. Knowledge revealed through this work will uncover the relevant genome locations that can be targeted for treatment. Furthermore, high-resolution 3D genome maps also encode unique patterns and signatures that in theory, can discriminate and diagnose exposure to chemical, biological, radiological, or nuclear events.

Publications

Journal Articles

*S. Bell, T. A., N. Velappan, C. D. Gleasner, G. Xie, S. R. Starkenburg, G. Waldo, S. Banerjee and S. N. Micheva-Viteva. Nonclassical autophagy activation pathways are essential for production of infectious Influenza A virus in vitro. 2022. *Molecular Microbiology*. **117** (2): 508-524. (LA-UR-20-30117 DOI: 10.1111/mmi.14865)

Biondi, T. C., C. P. Singer Kruse, S. I. Koehler, T. Kwon, W. L. K. M. Eng, Y. A. Kunde, C. D. Gleasner, K. T. You Mak, J. E. W. Polle, B. Hovde, E. R. Hanschen and S. R. Starkenburg. Assembly and analysis of the 100% complete, gapless, phased diploid genome of Scenedesmus obliquus UTEX 3031. Submitted to *Nucleic Acids Research*. (LA-UR-22-31391)

Lappala, A., C. Y. Wang, A. Kriz, H. M. Michalk, K. Tan, J. Lee and K. Y. Sanbonmatsu. 4D chromosome reconstruction elucidates the spatial reorganization of the mammalian X-chromosome. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-21-29486)

Rogers, D. H., C. J. N. Roth, C. Tauxe, J. T. Lee, K. Y. Sanbonmatsu, A. Lapalla and S. R. Starkenburg. Creating and Exploring Genome Structural Dynamics with the 4D Genome Browser and 4DGB Workflow. Submitted to *Nature Protocols*. (LA-UR-22-31631)

Tung, C., J. C. Miner, K. Y. Sanbonmatsu, P. W. Fenimore, W. M. Fischer and B. H. Mcmahon. Structure and function of the SARS-CoV-2 Spike protein during the fusion process. Submitted to *Journal of Biomolecular Structure & Dynamics*. (LA-UR-21-20482)

Reports

Job, V., W. L. K. M. Eng, C. J. N. Roth, T. Estrada, N. E. Lubbers, K. Y. Sanbonmatsu and C. R. Steadman. Relating Epigenetic Information to the Structure of DNAUsing Deep Learning – Preliminary Report. Unpublished report. (LA-UR-21-28663)

Presentation Slides

K. M. Eng, W. L., V. Job, C. J. N. Roth, C. R. Steadman, K. Y. Sanbonmatsu and S. R. Starkenburg. Correlation and Prediction of Epigenetic Data types; Machine learning lessons. Presented at *2021 Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27669)

Job, V. Relating Epigenetic Information to the Structure of DNA Using Deep Learning. Presented at *HPC Showcase*, Los Alamos, New Mexico, United States, 2021-08-11 - 2021-08-11. (LA-UR-21-27981)

Job, V. R., T. Estrada, V. Venu, C. J. N. Roth, N. E. Lubbers, C. R. Steadman and K. Y. Sanbonmatsu. Relating Epigenetic Information to the Structure of DNA Using Machine Learning. Presented at *HPC Intern Showcase*, Los Alamos, New Mexico, United States, 2022-08-11 - 2022-08-11. (LA-UR-22-28362)

Modl, D. G. Developments in the use of HTC Vive Pro Secure; Finally a headset we can use in our production work.. Presented at *Sandia's 3rd Annual XR Conference*, Albuquerque, New Mexico, United States, 2021-02-16 - 2021-02-18. (LA-UR-21-20987)

Rogers, D. H., K. Y. Sanbonmatsu and S. R. Starkenburg. 4DGenomeBrowser Prototype. . (LA-UR-21-22090)

Starkenburg, S. R. Bioscience & Genomics @ LANL. . (LA-UR-22-32020)

Starkenburg, S. R., T. C. Biondi, K. Y. Sanbonmatsu, C. P. Singer Kruse, E. R. Hanschen and B. Hovde. Advances in Algal Genomics. Presented at *Seq*, Santa Fe, New Mexico, United States, 2022-06-21 - 2022-06-21. (LA-UR-22-25747)

Steadman, C. R. Survive & Thrive: how epigenetics improves stress resilience. . (LA-UR-21-23296)

Venu, V. Pictures of Agilent tape station in HRL.. . (LA-UR-22-26254)

Posters

Job, V. R., C. J. N. Roth, V. Venu, T. Estrada, N. E. Lubbers, K. Y. Sanbonmatsu and C. R. Steadman. The correlation between accessible DNA and the epigenetic tag H3K27ac varies by chromosome. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-10. (LA-UR-23-22105)

Job, V., W. L. K. M. Eng, C. J. N. Roth, T. Estrada, N. E. Lubbers, S. R. Starkenburg, K. Y. Sanbonmatsu and C. R. Steadman. Relating Epigenetic Information to the Structure of DNA Using Deep Learning. . (LA-UR-21-28818)

N. Roth, C. J., S. N. Micheva-Viteva, V. Venu, A. Singhal, D. H. Rogers, C. R. Steadman, K. Y. Sanbonmatsu and S. R. Starkenburg. A 4D Genome Project: Elucidating the 3D genomic architecture in models of cellular infection and cellular development.. Presented at *Annual Sequencing, Finishing, and Analysis in the Future (SFAF) Conference*, Santa Fe, New Mexico, United States, 2022-06-21 - 2022-06-23. (LA-UR-22-25750)

Venu, V., C. J. N. Roth, S. N. Micheva-Viteva, S. H. Adikari, K. Y. Sanbonmatsu, S. R. Starkenburg and C. R. Steadman. Understanding the interplay between histone modifications and chromatin configuration in the human genome. Presented at *Cold Spring Harbor Conference : Genome organization and nuclear function*, Cold Spring Harbor, New York, United States, 2022-05-03 - 2022-05-07. (LA-UR-22-23778)

Venu, V., S. N. Micheva-Viteva, C. J. N. Roth, A. Singhal, C. Tauxe, D. H. Rogers, C. R. Steadman, K. Y. Sanbonmatsu and S. R. Starkenburg. A 4D Genome Project: Elucidating the 3D Genomic Architecture in Models of Cellular Infection and Development. Presented at *Annual Sequencing, Finishing,* *and Analysis in the Future (SFAF) Conference*, Santa Fe, New Mexico, United States, 2022-06-20 - 2022-06-22. (LA-UR-22-25674)

**Peer-reviewed*

Complex Natural and Engineered Systems

Directed Research
Continuing Project

Advanced Characterization to Enable Prediction of Actinide-Molten Salt Behavior

Marisa Monreal
20210113DR

Molten salts are fascinating to observe; they glow red-hot and flow like water, as seen in this photo of molten salt pouring into a glovebox furnace. Molten salts containing actinides are complex systems integral to both the next generation of nuclear energy and weapons production. This project addresses the need for an increased understanding of these systems; one that enables prediction of their behavior, a crucial capability that does not currently exist. Advanced characterization techniques in experiment and modeling, tailored to contend with these systems' challenging nature (radioactive, high-temperature) will be integrated to generate a validated actinide-molten salt predictive capability.

Project Description

Actinide-molten salts are complex systems integral to both the next generation of nuclear energy and weapons production. This project addresses the need for an increased understanding of these systems – one that enables prediction of their behavior, a crucial capability that does not currently exist. Our approach is to integrate innovative modeling methods and measurements of macroscale properties (e.g. density, viscosity, corrosivity) in order to create a robust predictive capability. This work will provide the fundamental basis for understanding factors that impact the efficiencies of the metal purification processes at the heart of the national weapons production mission. It will also advance the science and engineering knowledge that underpins the design and operation of the molten salt reactor, a next-generation nuclear energy reactor concept, addressing critical gaps currently holding back development of the technology. A suite of new capabilities for the advanced characterization of actinide-molten salts will result from this project. We expect to (1) produce highly accurate measurements and simulations of actinide-molten salt properties, (2) gain insight into local structure of actinide molten salts, one that helps explain observed macroscale property behavior, and (3) generate models with quantified uncertainty for a broad range of actinide-molten salt compositions.

Publications

Journal Articles

*Andersson, D. A. and B. W. Beeler. Ab initio molecular dynamics (AIMD) simulations of NaCl, UCl3 and NaCl-UCl3 molten salts. 2022. *Journal of Nuclear Materials*. **568**: 153836. (LA-UR-22-20387 DOI: 10.1016/j.jnucmat.2022.153836)

*Lhermitte, C. R., S. S. Parker, J. M. Jackson and M. J. Monreal. Communication-Mg2+/0 as a Reliable Reference Electrode for Molten Chloride Salts. 2021. *Journal of The Electrochemical Society*. **168** (6): 66501. (LA-UR-21-20290 DOI: 10.1149/1945-7111/ac0303)

*Parker, S. S., A. Long, C. Lhermitte, S. Vogel, M. Monreal and J. M. Jackson. Thermophysical properties of liquid chlorides from 600 to 1600\xc2\xa0K: Melt point, enthalpy of fusion, and volumetric expansion. 2022. *Journal of Molecular Liquids*. **346**: 118147. (LA-UR-21-22826 DOI: 10.1016/j.molliq.2021.118147)

*Vogel, S. C., D. A. Andersson, M. J. Monreal, J. M. Jackson, S. S. Parker, G. Wang, P. Yang and J. Zhang. Crystal Structure Evolution of UCl3 from Room Temperature to Melting. 2021. *JOM*. **73** (11): 3555-3563. (LA-UR-21-24639 DOI: 10.1007/s11837-021-04893-7)

Vogel, S. C., M. J. Monreal and A. P. Shivprasad. Materials for Small Nuclear Reactors and Micro Reactors, Including Space Reactors. 2021. *JOM*. **73** (11): 3497-3498. (LA-UR-21-28723 DOI: 10.1007/s11837-021-04897-3)

Wang, G., B. Li, P. Yang and A. D. R. Andersson. Ab-Initio Molecular Dynamics Simulations of Binary NaCl-ThCl4 and Ternary NaCl-ThCl4-UCl3 Molten Salts. Submitted to *Journal of Molecular Liquids*. (LA-UR-23-22328)

Yankey, J., J. Chamberlain, M. J. Monreal, J. M. Jackson and M. Simpson. UCl3 synthesis in molten LiCl-KCl and NaCl-MgCl2 via galvanically coupled uranium oxidation and FeCl2 reduction. Submitted to *Journal of Radioanalytical and Nuclear Chemistry*. (LA-UR-22-30400)

Conference Papers

R. Andersson, A. D. and B. Beeler. AB INITIO MOLECULAR DYNAMICS SIMULATIONS OF MOLTEN URANIUM CHLORIDE SALTS. Presented at *Fundamental Properties to Advance Molten Salt Reactor Technology Workshop*. (Richland, Washington, United States, 2022-03-28 - 2022-03-28). (LA-UR-21-31589)

Presentation Slides

R. Andersson, A. D. Modeling and Simulation of Actinide-Containing Molten Chloride Properties. . (LA-UR-21-21030)

R. Andersson, A. D. Ab Initio Molecular Dynamics Simulations of Actinide Molten Chloride Salts. Presented at *TMS Annual Meeting and Exhibition 2021*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-21786)

R. Andersson, A. D. Ab Initio Molecular Dynamics Simulations of Molten Uranium Chloride Salts. Presented at *Wisconsin Seminar*, Los Alamos, New Mexico, United States, 2021-09-28 - 2021-09-28. (LA-UR-21-29579)

R. Andersson, A. D., G. Wang, B. Li and P. Yang. Chromium Solution in Molten Uranium-Sodium Chloride Salts Investigated by Ab Initio Molecular Dynamics Simulations. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-19. (LA-UR-23-22518)

R. Andersson, A. D. and C. Jiang. Predicting thermodynamic and thermophysical properties of molten chloride salts from ab-initio and classical molecular dynamics simulations. Presented at *NEAMS telecon*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-29129)

Erickson, K. Synthesis of Actinide Halides: Year 2 Appraisal. . (LA-UR-23-20283)

Jackson, J. M. and M. J. Monreal. GAIN: Neutron Beam Dilatometry for Molten Salt Density Measurments. Presented at *NE-43 Molten Salt Chemistry PIs Meeting*, Virtual, New Mexico, United States, 2021-06-28 - 2021-06-29. (LA-UR-21-26025)

Kennedy, A. M., M. J. Monreal and K. Erickson. Analysis and quantification of molten chloride salt components for nonproliferation and accountability purposes. . (LA-UR-22-28232)

J. Lhermitte, C. R. Investigating the electrochemical behavior of uranium in molten chloride melts. . (LA-UR-23-21238)

J. Lhermitte, C. R. Investigating the electrochemical behavior of uranium in chloride molten salts. . (LA-UR-23-22316)

J. Lhermitte, C. R., S. S. Parker, J. M. Jackson and M. J. Monreal. Developing robust reference electrode chemistry for electrochemical corrosion experiments in actinide bearing molten salts. Presented at *Actinide Separations Conference*, Richland, Washington, United States, 2021-05-18 - 2021-05-20. (LA-UR-21-24855)

Long, A. M., S. C. Vogel, J. M. Jackson, M. J. Monreal and S. S. Parker. Dilatometry via Neutron Radiography. . (LA-UR-20-29587)

Long, A. M., S. C. Vogel, J. R. Torres, D. T. Carver, S. S. Parker, M. J. Monreal and J. M. Jackson. Neutron Imaging at LANSCE: Characterizing Materials for the Next Generation of Nuclear Reactor Designs. Presented at *Computational Imaging XXI*, San Fransico, California, United States, 2023-01-16 - 2023-01-19. (LA-UR-23-20813)

Long, A. M., S. C. Vogel, J. R. Torres, S. S. Parker, M. J. Monreal, J. M. Jackson, D. T. Carver, K. J. Mcclellan, J. R. Angell, T. Balke, L. Capriotti, A. E. Craft, J. M. Harp, P. Hosemann, E. J. Larson, D. Schaper, B. E. Wohlberg, C. A. Bouman and A. S. Tremsin. Characterizing Materials for Next Generation

Nuclear Reactor Designs with Neutron Imaging at LANSCE. . (LA-UR-23-22834)

Long, A. M., T. Balke, D. T. Carver, J. M. Jackson, S. C. Vogel, M. J. Monreal, S. S. Parker, E. P. Luther, A. P. Shivprasad, H. R. Trellue, D. Schaper, A. S. Tremsin, K. J. Mcclellan, B. E. Wohlberg, J. Angell, L. Capriotti, A. E. Craft, J. Harp, P. Hosemann, E. J. Larson and A. Losko. Neutron Imaging at LANSCE: Characterizing Nuclear Materials for Next Generation Reactor Designs. Presented at *TMS2021*, Virtual, New Mexico, United States, 2021-03-14 - 2021-03-18. (LA-UR-21-22273)

Long, A. M., T. Balke, S. C. Vogel, M. J. Monreal, J. M. Jackson, S. S. Parker, E. P. Luther, A. P. Shivprasad, H. R. Trellue, A. S. Tremsin, A. S. Losko, J. R. Torres, V. K. Mehta and D. T. Carver. NEUTRON RADIOGRAPHY AT LANSCE: Interrogation and Characterization of Materials for Next Generation Nuclear Reactor Designs. Presented at *Twelfth International Conference on Methods and Applications of Radioanalytical Chemistry*, KAILUA-KONA, Hawaii, United States, 2022-04-04 - 2022-03-11. (LA-UR-22-23074)

Monreal, M. J. LANL Actinide-Molten Salt Research Capability. . (LA-UR-22-23319)

Monreal, M. J. Thermochemical and Thermophysical Property Database Development at LANL. Presented at *Molten Salt Reactor Campaign Review (Virtual Meeting, on Teams)*, Richland, Washington, United States, 2022-04-26 - 2022-04-27. (LA-UR-22-23878)

Monreal, M. J. The LANL Molten Salt Research Capability: 2022 Status Update. Presented at *Molten Salt Reactor Workshop*, Oak Ridge, Tennessee, United States, 2022-10-11 - 2022-10-12. (LA-UR-22-30476)

Monreal, M. J. Actinide-Molten Salt Research at LANL: Innovating for the Next Generation of Nuclear Energy. . (LA-UR-23-23249)

Monreal, M. J. and J. M. Jackson. Molten Salt Research at Los Alamos National Laboratory. Presented at *Molten Salt Reactor Workshop*, Oak Ridge, Tennessee, United States, 2020-10-14 - 2020-10-15. (LA-UR-20-28152)

Parker, S. S., N. M. Abdul-Jabbar, A. M. Long, A. C. Strzelecki, S. C. Vogel, A. D. R. Andersson, C. R. J. Lhermitte, S. C. Mann, A. B. Gomez, H. Xu, J. M. Jackson and M. J. Monreal. Thermophysical Properties of Liquid Halides. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-02-23. (LA-UR-23-22070)

Parker, S. S., N. M. Abdul-Jabbar, J. M. Jackson and M. J. Monreal. Volumetric Expansion of Molten Chlorides by Conventional Pushrod Dilatometry. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kailua-Kona, Hawaii, United States, 2022-04-04 - 2022-04-08. (LA-UR-22-23948)

Parker, S. S., S. C. Mann, J. M. Jackson and M. J. Monreal. Determination of the Eutectic Composition in NaCl + MgCl2. . (LA-UR-21-29396)

Patenaude, H. K., C. R. J. Lhermitte, N. Damjanovic, J. Rakos, S. D. Branch, M. J. Monreal and C. A. Rusinek. Electrochemical Characterization of Molten Salt Fuel System with Boron-Doped Diamond. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-23. (LA-UR-23-22889)

Vogel, S. C., A. D. R. Andersson, M. J. Monreal, J. M. Jackson, S. S. Parker, G. Wang, P. Yang, B. Khaykovich and J. Zhang. Neutron Scattering Characterization of UCl3 from Room Temperature to Melting. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-23. (LA-UR-23-22572)

Vogel, S. C., A. D. R. Andersson, M. J. Monreal, J. M. Jackson, S. S. Parker, G. Wang, P. Yang and J. Zhang. Neutron Pair Distribution Function Studies of Actinide-Molten Salts. Presented at *Actinide Separations Conference*, virtual, New Mexico, United States, 2021-05-18 - 2021-05-20. (LA-UR-21-24556)

Yankey, J., J. Chamberlain, M. F. Simpson, M. J. Monreal and J. M. Jackson. Chlorination of U Metal with FeCl2 in LiCl-KCl and NaCl-MgCl2. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-20. (LA-UR-23-22917)

Posters

Li, B., E. R. Batista and P. Yang. Multi-scale Modeling of Nuclear Energy Materials. Presented at *Kavli Frontiers of Science 19th Chinese American Symposium*, Irvine, California, United States, 2022-07-08 - 2022-07-10. (LA-UR-22-26617)

Long, A. M., D. T. Carver, J. M. Jackson, M. J. Monreal, S. S. Parker and S. C. Vogel. Using Neutrons to Measure Densities of Molten Salts. . (LA-UR-23-21939)

Monreal, M. J., J. M. Jackson, S. C. Vogel, B. Khaykovich and A. D. R. Andersson. Investigating the Local Structure of Actinide-Molten Salts Using Pair-Distribution Function Analysis. Presented at *Plutonium Futures*, Avignon, France, 2022-09-26 - 2022-09-26. (LA-UR-22-29835)

Parker, S. S., A. B. Gomez, S. C. Mann, N. M. Abdul-Jabbar, J. M. Jackson, S. C. Vogel, A. M. Long and M. J. Monreal. Thermophysical Properties of Liquid Actinide Halides. Presented at *Plutonium Futures*, Avignon, France, 2022-09-26 - 2022-09-30. (LA-UR-22-29869)

Yankey, J., M. J. Monreal, J. M. Jackson, S. S. Parker, S. Choi and M. Simpson. Measurement of Vapor Pressure of UCl3 in NaCl-MgCl2-UCl3 via Transpiration Experiments. Presented at *Minerals, Metals & Materials Society (TMS) Annual*

Meeting and Exhibition, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-21475)

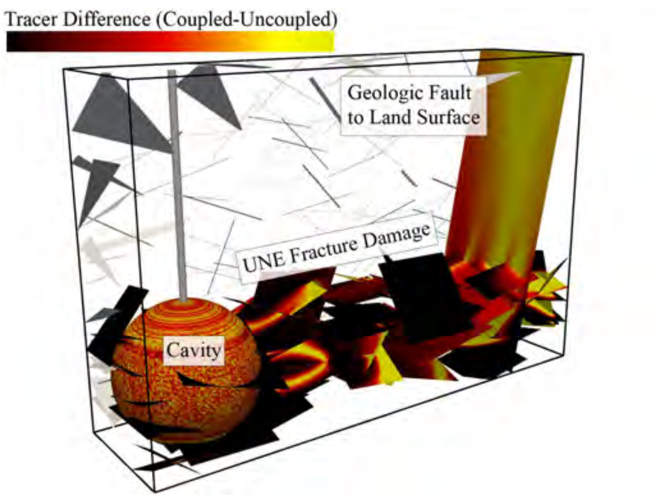
Other

Li, B., E. R. Batista and P. Yang. Dataset of Understanding the Structural, Dynamical, Chemical and Thermophysical Properties of Molten Chlorides for Molten Salt Reactors using Electronic Structure Methods. Dataset. (LA-UR-23-20714)

**Peer-reviewed*

Discovering Radioactive Gas Transport Feedbacks from Underground Nuclear Explosions: Predictions Validated by Observations

Philip Stauffer
20220019DR



Underground nuclear explosions drive gases from the nuclear cavity through damaged rock, toward existing faults in the earth. By including pressure driven feedbacks on fault permeability in 3 dimensional simulations, predictions of gas migration generate increased flow to the land surface (yellow). Understanding complex feedbacks that link engineered and natural systems will allow us to better design underground tests as part of US test readiness and increase our understanding of leakage from foreign nuclear tests.

Project Description

Radioactive gases emerging from the ground after a subsurface nuclear detonation allow analysts to positively identify subsurface nuclear testing. This diagnostic can be used in combination with other methods such as seismic analysis to provide confidence in definitively discriminating between chemical and nuclear explosions. Predicting radioactive gas migration requires simulation of multiple phenomena, beginning with a nuclear detonation and expanding fireball of gases that destroys underground facilities. The blast generates radial fractures, activates natural fractures, and ultimately can inject gas far into the surrounding geology. The current practice for predicting Underground Nuclear Explosion (UNE) gas release uses simplified physics, resulting in radioactive gas release predictions that are missing key feedbacks that compromise potential future US test containment or suspected UNEs detection. Similarly, current containment science simulations at Los Alamos National Laboratory and Lawrence Livermore National Laboratory rely on previous generation couplings (e.g., fixed fracture orientations, two-dimensional, and continuum approximations) that have limited feedbacks. Our work will reduce uncertainty in gas transport predictions, advancing United States national objectives in containment science and underground nuclear explosion detection and characterization.

Publications

Journal Articles

Andrews, E., J. D. Hyman, M. R. Sweeney, S. Karra, J. D. Moulton and A. Navarre-Sitchler. Fracture intensity impacts on reaction front propagation and mineral weathering in three-dimensional fractured media. Submitted to *Water Resources Research*. (LA-UR-22-20567)

Dentz, M. and J. D. Hyman. The hidden structure of hydrodynamic transport in random fracture networks. Submitted to *Journal of Fluid Mechanics*. (LA-UR-23-20055)

Hyman, J. D., A. Navarre-Sitchler, E. M. Andrews, M. R. Sweeney, S. Karra, J. W. Carey and H. S. Viswanathan. Characterizing the influence of fractures network structure on apparent dissolution rates. Submitted to *Geophysical Research Letters*. (LA-UR-22-23817)

Hyman, J. D., M. R. Sweeney, C. W. Gable, D. Svyatsky, K. Lipnikov and J. D. Moulton. Flow and Transport in Three-Dimensional Discrete Fracture Matrix Models using Mimetic Finite Differencing on a Conforming Multi-Dimensional Mesh. Submitted to *Journal of Computational Physics*. (LA-UR-21-31458)

Hyman, J. D., M. R. Sweeney, C. W. Gable, J. C. Krotz and J. Restrepo. Maximal Poisson-disk Sampling for Variable Resolution Conforming Delaunay Mesh Generation: Applications for Three-Dimensional Discrete Fracture Networks and the Surrounding Volume. Submitted to *Journal of Computational and Applied Mathematics*. (LA-UR-21-31456)

Hyman, J. D., M. R. Sweeney, C. W. Gable, J. C. Krotz and J. Restrepo. Maximal Poisson-disk Sampling for Variable Resolution Conforming Delaunay Mesh Generation: Applications for Three-Dimensional Discrete Fracture Networks and the Surrounding Volume. Submitted to *Journal of Computational and Applied Mathematics*. (LA-UR-21-24804)

Lei, Z., A. Munjiza, E. Rougier, E. E. Knight and C. R. Bradley. AXISYMMETRIC FDEM FORMULATION FOR LARGE DEFORMATION SOLIDS. Submitted to *International Journal for Numerical Methods in Engineering*. (LA-UR-22-30243)

Lei, Z., A. Munjiza, E. Rougier, E. E. Knight and C. R. Bradley. AXISYMMETRIC FDEM FORMULATION FOR LARGE DEFORMATION SOLIDS. Submitted to *International Journal for Numerical Methods in Engineering*. (LA-UR-22-30924)

Pachalieva, A. A., M. R. Sweeney, H. S. Viswanathan, E. Stein, R. Leone and J. D. Hyman. Impact of artificial topological changes on flow and transport through fractured media due to mesh resolution. Submitted to *Computational Geosciences*. (LA-UR-23-20307)

Strait, J. D., K. R. Moran, J. D. Hyman, P. H. Stauffer, H. S. Viswanathan and M. R. Sweeney. Fracture Network Flow Prediction with Uncertainty using Physics-Informed Graph Features. Submitted to *Computational Geosciences*. (LA-UR-22-24994)

*Viswanathan, H. S., J. Ajo-Franklin, J. T. Birkholzer, J. W. Carey, Y. Guglielmi, J. D. Hyman, S. Karra, L. J. Pyrak-Nolte, H. Rajaram, G. Srinivasan and D. M. Tartakovsky. From Fluid Flow to Coupled Processes in Fractured Rock: Recent Advances and New Frontiers. 2022. *Reviews of Geophysics*. **60** (1): e2021RG000744. (LA-UR-21-28244 DOI: 10.1029/2021RG000744)

Yoon, S., J. D. Hyman, W. S. Han and P. Kang. Effects of dead-end fractures on non-Fickian transport in three-dimensional discrete fracture networks. Submitted to *Water Resources Research*. (LA-UR-22-28752)

Conference Papers

Huang, Y., Z. Lei, E. Rougier, B. J. Euser, A. M. Padilla and E. E. Knight. Boundary condition effect on 3-point bending test via FDEM. Presented at *57th US Rock Mechanics/ Geomechanics Symposium*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-06-28). (LA-UR-23-22438)

Huang, Y., Z. Lei, K. Lipnikov, J. D. Moulton, M. R. Sweeney, J. D. Hyman, E. E. Knight and P. H. Stauffer. Modeling Coupled Thermo-Hydro-Mechanical-Chemical Processes in Subsurface Geological Media. Presented at *57th US Rock Mechanics/Geomechanics Symposium*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-06-28). (LA-UR-23-22367)

Li, W., C. W. Neil, P. H. Stauffer, J. W. Carey, M. Meng and L. P. Frash. Characterization of Gas Transport in Fractured Rocks for Underground Nuclear Explosion Detection. Presented at *57th US Rock Mechanics / Geomechanics Symposium*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-06-28). (LA-UR-23-21958)

Reports

Berry, D., J. Kath, S. Lodhy, A. Ly, Y. Shi, A. Percus, J. D. Hyman, K. R. Moran, P. H. Stauffer, J. D. Strait, M. R. Sweeney and H. S. Viswanathan. Learning Gas Transport through Fracture Networks from Multi-Fidelity Data. Unpublished report. (LA-UR-22-20660)

Berry, D., J. Kath, S. Lodhy, A. Ly, Y. Shi, A. Percus, J. D. Hyman, K. R. Moran, P. H. Stauffer, J. D. Strait, M. R. Sweeney and H. S. Viswanathan. Learning Gas Transport through Fracture Networks from Multi-Fidelity Data. Unpublished report. (LA-UR-22-29932)

Presentation Slides

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Hyman, J. D., A. Sitchler, E. Andrews, M. R. Sweeney, S. Karra, J. W. Carey and H. S. Viswanathan. A Geo-structurally Based Correction Factor for Apparent Dissolution Rates in Fractured Media: AGU Presentation. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32654)

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Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. Algorithm Aspects of the Combined Finite-Discrete Element Method: An Overview. Presented at *Workshop "FDEM-2022 - Modeling innovations and numerical experiments in geomechanics"*, Toronto, Canada, 2022-12-09 - 2022-12-09. (LA-UR-22-32693)

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Strait, J. D. Discussion for "Advances in Topological and Geometric Data Analysis" (JSM 2022). Presented at *Joint Statistical Meeting*, Washington, District Of Columbia, United States, 2022-08-07 - 2022-08-11. (LA-UR-22-28325)

Viswanathan, H. S., J. W. Carey, L. P. Frash, J. D. Hyman, Q. Kang, E. Rougier and G. Srinivasan. A multi-scale experimental and machine learning enabled simulation approach for fractured subsurface systems. Presented at *CouFrac 2022*, Berkeley, California, United States, 2022-11-14 - 2022-11-16. (LA-UR-22-31929)

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Li, W., C. W. Neil, P. H. Stauffer, J. W. Carey and M. Meng. Investigation of Gas Transport for Underground Nuclear Explosion Detection Based on Triaxial Direct-Shear Tests. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32339)

Neil, C. W., W. Li, J. W. Carey, P. H. Stauffer and H. S. Viswanathan. Noble gas transport in the subsurface: Volatiles as a signature of nuclear detonation. Presented at *Volatiles from Source to Surface: A GeoPRISMS Workshop*, Bozeman, Montana, United States, 2022-05-23 - 2022-05-26. (LA-UR-22-24421)

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Stansberry, A. R., W. Gao, L. Gianuca, J. D. Hyman, E. E. Knight, T. Kong, J. Lee, Z. Lei, K. R. Moran, A. Percus, K. Sheldon, J. D. Strait, M. R. Sweeney, H. S. Viswanathan and P. H. Stauffer. Gas Transport in Fractured Rocks Resulting from Underground Nuclear Explosions: Exploring the Damage-Permeability Relationship. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32638)

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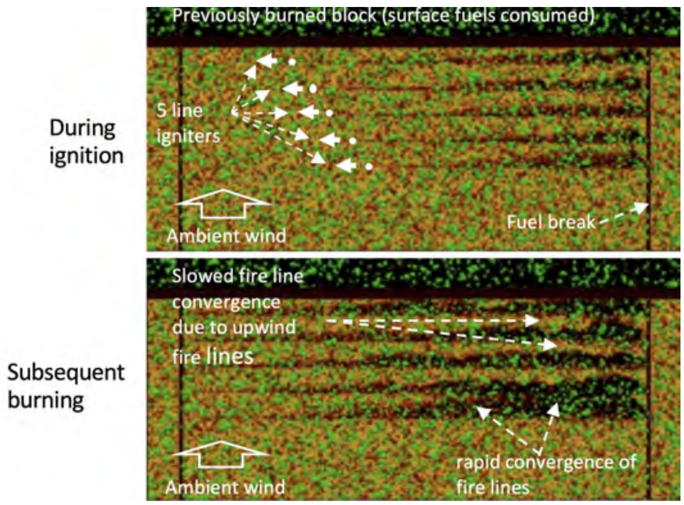
**Peer-reviewed*

Fighting Fire with Fire: Enabling a Proactive Approach to Wildland Fire

Rodman Linn
20220024DR



QUIC-Fire simulations of a prescribed fire at Eglin Air Force Base. This prescribed fire simulation illustrates the common use of multiple ignition lines (in this case by 5 igniters moving in a staggered pattern from right to left). The ignition patterns harnesses the interaction between the fire and the atmosphere to achieve desired fire effects for wildfire risk reduction and ecologic sustainability. These coupled fire/atmosphere simulations result in realistic heterogeneous spread rates between the upwind and downwind fire lines and highlight the importance of these feedbacks. The project aims to develop a framework for simulations of prescribed fire scenarios to select optimal treatments to meet fire-risk and ecosystem management objectives.

Project Description

This work will provide a critical science basis and an integrated tool supporting a proactive approach to wildland fire, a growing national problem that threatens communities and critical infrastructure. It has direct ties to national security (Department of Homeland Security (DHS), Department of Defense (DoD), and Weapon effects) and Los Alamos National Laboratory's Climate Initiative for National Security (climate change and proactive mitigation options). Through this work we will catalyze a new proactive trajectory in wildfire management through Rx fire application by integrating our unparalleled expertise in fire modeling, data analysis, and high-performance computing. Our approach will directly enhance decision-support for the Los Alamos site management, Los Alamos neighbors, and existing research and land agency partners. This effort is very will aligned with DoD's land management requirements and thus can help improve the resilience of DoD bases to wildland fire. Prescribed fire will reducing the risk of severe destruction due to terrorist instigated fire events and help harden our communities and infrastructure from natural and anthropogenic fire events. Three-dimensional fuels mapping capability and smoke and fire modeling are critical to anticipation of fire as a potential non-nuclear or nuclear weapon effect.

Publications

Journal Articles

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Robinson, D. J., S. Brambilla, M. J. Brown, P. T. Conry, B. Quaife and R. R. Linn. QUIC-URB and QUIC-fire extension to complex terrain: Development of a terrain-following coordinate system. 2022. *Environmental Modelling & Software*. 105579. (LA-UR-22-23520 DOI: 10.1016/j.envsoft.2022.105579)

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Atchley, A. L. IC Progress Report ViewGraphs. . (LA-UR-23-23256)

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Brambilla, S., D. J. Robinson, A. J. Josephson, V. G. Narayanan, N. Duboc, M. A. Nelson, M. J. Brown and R. R. Linn. Smoke in QUIC-Fire and QUIC-SMOKE. Presented at *Wildland Fire Canada Conference*, Edmonton, Canada, 2022-10-31 - 2022-11-04. (LA-UR-22-30979)

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Linn, R. R. Integrated Modeling to Support Prescribed Fire. Presented at *National Prescribed Fire Assessment*, Albuquerque, New Mexico, United States, 2022-05-09 - 2022-05-12. (LA-UR-22-32702)

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Linn, R. R. Wildland fire modeling: context, applications, and opportunities. Presented at *President*, virtual, New Mexico, United States, 2022-03-24 - 2022-03-24. (LA-UR-22-32703)

Linn, R. R. Coupled Fire-Atmosphere (CFA) tools: opening doors from fire research to prescribed fire applications. Presented at *9th International Fire Ecology and Management Congress*, Virtual presentation, New Mexico, United States, 2021-11-01 - 2021-12-03. (LA-UR-22-32684)

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McDanold, J. S. DUET: Distribution of Understory fuels using Elliptical Transport. Presented at *RIT Work-in-progress Presentation*, Rochester, New York, United States, 2021-11-15 - 2021-11-15. (LA-UR-21-31278)

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McDanold, J. S. Trees Mixed With Fire. Presented at *LANL Virtual Wildfire Simulation and Visualization Camp*, Los Alamos, New Mexico, United States, 2022-06-06 - 2022-06-17. (LA-UR-22-25364)

McDanold, J. S. Mathematical Modeling of Tree Litter Dispersal. Presented at *Grand Valley State University Seminar Series*, Allendale Charter Township, Michigan, United States, 2022-09-23 - 2022-09-23. (LA-UR-22-29807)

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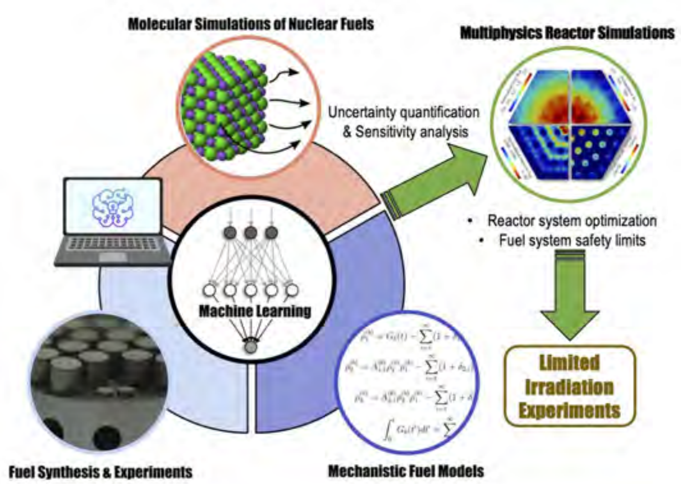
Killebrew, A. J. NMFD_FIA_names_FIA_Moisture_AllData_EXPORT. Dataset. (LA-UR-23-20229)

**Peer-reviewed*

Accelerating Nuclear Fuel Qualification through Integrated Multiscale and Multiphysics Models

Tammie Gibson
20220053DR



The developed AFQ framework leverages machine learning to fuse small datasets with input from atomic scale simulations, mechanistic fuel performance models, experiment, and reactor simulations to provide a unified model of swelling and fission gas behavior in nuclear fuel with quantified uncertainty. New models are integrated with engineering-scale multiphysics reactor models to define fuel performance safety margins. Advanced modeling and simulation accelerate the licensing timeline by limiting integral experiments needed for qualification.

Project Description

The slow timeline and high cost of nuclear fuel qualification prevent development of new fuels and reactor technologies. The Nuclear Regulatory Commission has expressed interest in integrating advanced modeling and simulation into the qualification process, a concept known as Accelerated Fuel Qualification (AFQ). This project develops an AFQ framework using data science to couple disparate models and targeted experiments to validate models and reduce uncertainty, reducing the quantity of irradiation tests. We expect to develop accurate mechanistic models of fuel swelling. The developed mechanistic models will be applied in reactor simulations that ultimately define fuel safety margins within specific reactor conditions, and quantify sources of uncertainty that most strongly influence fuel performance predictions. We can then determine whether experiments are required to further reduce the uncertainty or if the existing uncertainty is acceptable from a qualification standpoint. The AFQ framework will have immediate impact on advanced reactor fuels, can benefit future reactor concepts as well as the existing reactor fleet, and will inform the direction of future targeted irradiation experiments. The work will benefit several Department of Energy- Nuclear Energy programs and addresses the identified need of the Los Alamos National Laboratory integrated nuclear energy and materials initiative targeting advanced fuel qualification with uncertainty estimations.

Publications

Journal Articles

D. Cooper, M. W., J. T. Rizk, C. Matthews, V. Kocevski, G. T. Craven, T. R. Gibson and A. D. R. Andersson. Simulations of self- and Xe diffusivity in uranium mononitride including chemistry and irradiation effects. Submitted to *Journal of Nuclear Materials*. (LA-UR-23-21397)

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Miller, Z. A., M. Fratoni and V. K. Mehta. Thermomechanical Limitations of Uranium Mononitride. Presented at *Nuclear and Emerging Technologies for Space (NETS)*. (Idaho Falls, Idaho, United States, 2023-05-07 - 2023-05-11). (LA-UR-23-22369)

Reports

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Presentation Slides

R. Andersson, A. D. Multiscale Modeling Update. Presented at *5th AFQ Workshop*, Washington DC, New Mexico, United States, 2023-01-26 - 2023-01-26. (LA-UR-23-20765)

R. Andersson, A. D., C. Matthews, J. T. Rizk, R. T. Perriot, M. W. D. Cooper, X. Liu and C. R. Stanek. Cluster dynamics simulations of point defects and fission gas evolution in irradiated ceramic nuclear fuels. Presented at *Materials Science & Technology (MS&T) Technical Meeting*, Pittsburgh, Pennsylvania, United States, 2022-10-09 - 2022-10-09. (LA-UR-22-30820)

Craven, G. T. Parameter optimization in CENTIPEDE model. . (LA-UR-23-20550)

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Matthews, C., M. W. D. Cooper, J. T. Rizk, V. K. Mehta and A. D. R. Andersson. Physics-based model for swelling in U(C,N) nuclear fuel and macro-scale reactor modeling. Presented at *LDRD project kick-off meeting*, Los Alamos, New Mexico, United States, 2021-10-27 - 2021-10-27. (LA-UR-21-30696)

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Nelson, T. R. LDRD-DR: Accelerating Nuclear Fuel Qualification through Integrated Multiscale and Multiphysics Models. . (LA-UR-22-25772)

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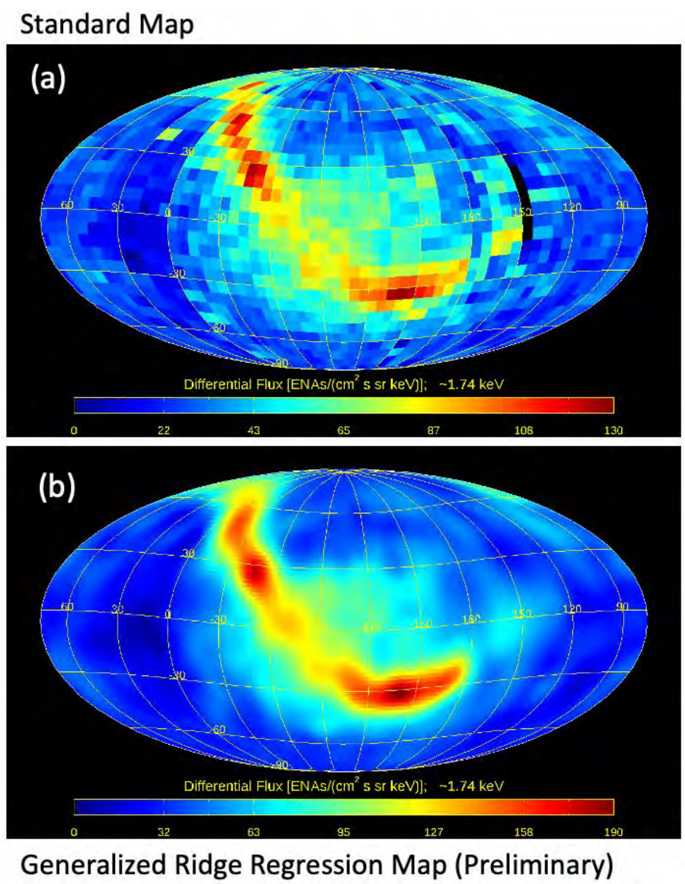
Alzate Vargas, L. L., E. L. Stippell, K. N. Subedi, B. T. Nebgen, J. S. Smith, S. Tretiak, T. R. Gibson, R. M. Tutchton, M. W. D. Cooper and R. A. Messerly. Machine learning interatomic potentials for accelerated nuclear fuel qualification. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21676)

**Peer-reviewed*

Discovering the Structure and Dynamics of the Sun-Interstellar Medium System

Daniel Reisenfeld
20220107DR



The NASA Interstellar Boundary Explorer (IBEX) mission has made a number of groundbreaking advances in our understanding of the interstellar boundary by imaging the boundary through detection of energetic neutral atoms (ENAs) (a). However, the ability to make further breakthroughs is limited by the quality of the standard IBEX data products. This project will carry out new discovery science by applying advanced statistical imaging techniques to build higher resolution, statistically robust ENA maps (b), as well as incorporating advanced theoretical modeling of the heliosheath-interstellar medium interaction. [Image credits: (a) NASA/IBEX, (b) Los Alamos National Laboratory]

Project Description

This is a project to understand the heliosphere's interstellar boundary, the region of space that defines the edge between the Sun's magnetic and particle influence and the interstellar medium. We will apply innovative low-signal, high-background statistical imaging and statistical learning techniques to greatly enhance the scientific quality of images of the interstellar boundary made by the National Aeronautics and Space Administration's (NASA) Interstellar Boundary Explorer (IBEX). This will allow us to carry out new discovery science, and it will complement Los Alamos National Laboratory's hardware role on the follow-on mission to IBEX, the NASA Interstellar Mapping and Acceleration Probe (IMAP), by building new science capability, positioning Los Alamos for a leadership role in IMAP science just in time for the IMAP launch in 2025. This project address national security issues in two ways: First, the interstellar boundary acts as a barrier to harmful galactic cosmic rays (GCRs) which are a threat to national space assets and human spaceflight. It is important to understand how the interstellar boundary modulates GCRs and under what conditions the barrier may weaken and lead to an increased GCR threat. Second, the statistical science advances made in this project will be applied (as part of this project) to the Space-based Nuclear Detonation Detection (SNDD) domain.

Publications

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Moran, K. R. Fast Approximate Bayesian Gaussian Process Regression. Presented at *2022 International Society for Bayesian Analysis World Meeting*, Montreal, Canada, 2022-06-27 - 2022-07-01. (LA-UR-22-25861)

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Reisenfeld, D. B., H. O. I. Funsten, M. Bzowski, M. A. Kubiak, J. Heerikhuisen, D. J. McComas, N. A. Schwadron, J. Sokol, A. Zimorino, P. Janzen and E. Zirnstein. Mapping the Boundary of the Heliosphere in 3D from IBEX. Presented at *SHINE*, Honolulu, Hawaii, United States, 2022-06-27 - 2022-07-01. (LA-UR-22-25951)

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**Peer-reviewed*

Radiation Belt Remediation: A Complex Engineered System (RBR-ACES)

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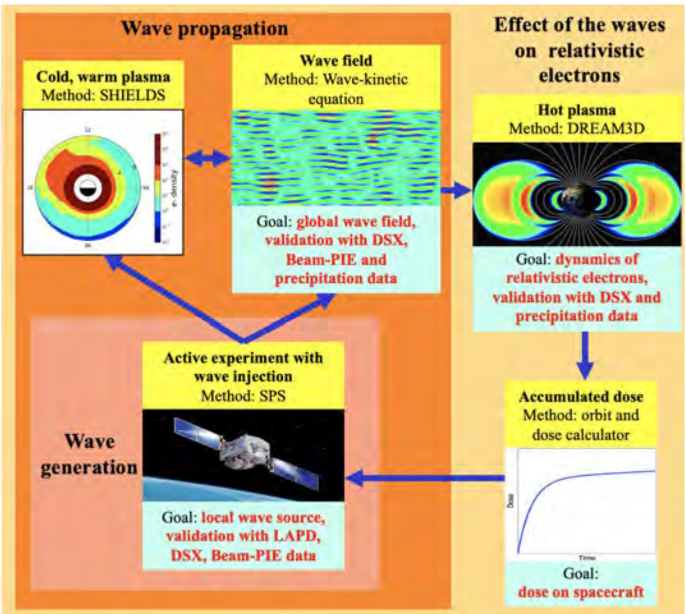
20200073DR



RBR-ACES is an end-to-end, validated modeling framework to assess if space-based injection of electromagnetic plasma waves can remediate an artificial radiation belt of relativistic electrons created by a high-altitude nuclear explosion. The goal is to return the space environment to pre-explosion levels sufficiently fast to protect space assets and replenish assets that might have been lost.

Project Description

A high-altitude nuclear explosion (HANE) at low latitudes (such as in North Korean nuclear test) creates a high-intensity, long-lasting artificial radiation belt of relativistic electrons that would damage all low-Earth-orbit satellites not specifically designed against a nuclear event and would cripple United States national security capabilities for years. This project will develop an end-to-end, validated, computational framework to estimate the feasibility of a space-based radiation belt remediation system based on the injection of electromagnetic plasma waves and aimed at returning the post-HANE environment to levels that are safe for our space infrastructure as quickly as necessary (i.e. within less than a month).

Technical Outcomes

The project successfully developed the RBR-ACES end-to-end modeling framework to assess the ability of using space-based injection of electromagnetic plasma waves to remediate an artificial radiation belt created by a high-altitude nuclear explosion. A strong validation effort with laboratory experiments and space-based experiments and observations was also successfully performed to build confidence in the framework. RBR-ACES results point to the importance of optimizing a radiation belt remediation system to minimize its power requirements.

Publications

Journal Articles

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Reports

Cunningham, G. S. and J. Ripoll. Effects of whistler waves in the near-Earth environment. Unpublished report. (LA-UR-22-29171)

Delzanno, G. L. Notes on radiated power from a modulated beam. Unpublished report. (LA-UR-21-28197)

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Presentation Slides

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**Peer-reviewed*

Directed Plant-Microbiome Evolution for Food and Biofuel Security

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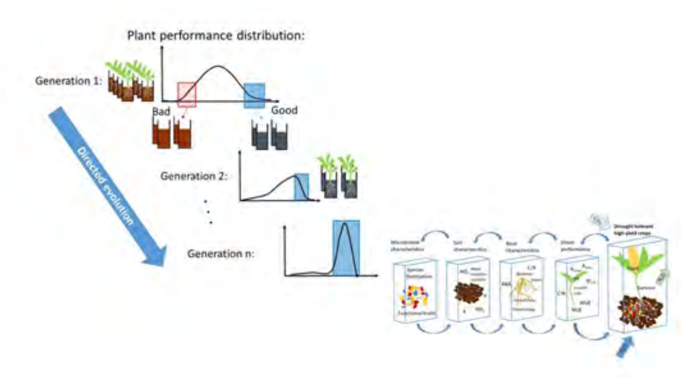

Improving plant drought tolerance is essential for matching the future food and biofuel needs. Optimizing the soil microbiome to support plant productivity under stress has been suggested as a solution, but developing microbiomes that improve plant drought tolerance has proven hard. This project is developing methods to produce microbiomes that improve plant drought tolerance using a directed evolution approach combined with plant, soil and microbiome characterization and machine learning to resolve this challenge.

Project Description

This work addresses the national and global security challenge of stability of food and biofuel production under increasingly unpredictable and, in many cases, deleterious climate by developing new, relatively easy, cheap and fast methods for producing beneficial microbiomes to improve crop production. Capabilities developed in this project have broad biotechnology applications to resolve emerging challenges in health, food, and biofuel security, and environmental stability, as well as proliferation detection and bioremediation. With our technology it is possible to develop new microbial or vegetation bioindicators for pollution or effluent detection. Agriculture as the largest user of fresh water in global scale is tightly linked with the Department of Energy (DOE) mission on energy security, and its global and national importance is increasing with population growth. New biotechnology developed in this project is at the cutting edge of the field, and allows leaps forward to utilize microbiomes to benefit human kind, but it also introduces risks of malevolent use. It is important for National Nuclear Security Administration (NNSA) global security mission to be in the fore front of this emerging technology to promote beneficial applications while also informing risk assessment of mis-use.

Technical Outcomes

The team demonstrated, for the first time, that directed plant-microbiome evolution (host-mediated microbiome engineering) can alter plant physiological traits related to drought tolerance. Via directed evolution process, the team successfully produced two microbial phenotypes from a pine forest microbiome that differently influence stomatal closure point under drought in maize. Additionally, machine learning methods showed that microbiomes affecting plant nitrogen use and cell wall formation are the key to altering stomatal closure point.

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Sevanto, S. A. Vegetation-climate interactions in the changing world: What determines who survives, and what can we do about it. . (LA-UR-21-21276)

Sevanto, S. A. Food security in a changing world. Presented at *CNES review*, Los Alamos, New Mexico, United States, 2021-05-05 - 2021-05-07. (LA-UR-21-23535)

Sevanto, S. A. Phloem transport under drought. . (LA-UR-21-24203)

Sevanto, S. A. Climate solutions bridging environmental physics and design. Presented at *Vision 2020(1), AIA Western Mountain Region Summit*, Albuquerque, New Mexico, United States, 2021-10-01 - 2021-10-01. (LA-UR-21-29414)

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Sevanto, S. A. Virtual tour of LANL plant science capabilities. . (LA-UR-23-20188)

Sevanto, S. A., K. R. Carter, E. R. Moore, A. C. Nachtsheim, A. Kim, J. M. Mitchell, L. T. Dickman, J. P. Heneghan, A. J. Sabella, C. M. Anderson-Cook, J. M. Heikoop, N. E. Lubbers, D. Musa, S. Negi, B. D. Newman, S. N. Twary, C. M. Yeager, L. Comas, C. R. Steadman, C. R. Kuske, C. Gehring, M. B. N. Albright and J. M. Dunbar. Directed plant-microbiome evolution to improve plant drought tolerance. Presented at *University of Helsinki, Forest Sciences Seminar*, Helsinki, Finland, 2022-09-02 - 2022-09-02. (LA-UR-22-28509)

Sevanto, S. A., K. R. Carter, E. R. Moore, A. C. Nachtsheim, A. Kim, J. M. Mitchell, L. T. Dickman, J. P. Heneghan, A. J. Sabella, C. M. Anderson-Cook, J. M. Heikoop, N. E. Lubbers, D. Musa, S. Negi, B. D. Newman, S. N. Twary, C. M. Yeager, L. Comas, C. R. Steadman, M. B. N. Albright and J. M. Dunbar. Can plant-microbiome interactions be harnessed to support food security and carbon sequestration?. Presented at *ISCRAES2022*, Dublin, Ireland, 2022-08-28 - 2022-08-31. (LA-UR-22-28508)

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Posters

Carter, K. R., D. Musa, J. P. Heneghan, E. R. Lathrop, L. T. Dickman, S. N. Twary, J. M. Dunbar and S. A. Sevanto. Controls of corn stomatal closure point across ontogenic stages, generations, and microbiomes. Presented at *Ecological Society of America Annual Conference*, Online, New Mexico, United States, 2020-08-03 - 2020-08-06. (LA-UR-20-25430)

Carter, K. R., J. M. Mitchell, C. M. Yeager, L. T. Dickman, E. A. Gomez, E. M. Rodriguez, J. P. Heneghan, B. D. Newman, E. R. Moore, L. Comas, R. J. Harris, N. E. Lubbers, O. C. Marina, A. C. Nachtsheim, G. B. Perkins, C. R. Steadman and S. A. Sevanto. Drought and microbiome effects on maize growth and root metabolomics. Presented at *Ecological Society of America Annual Meeting*, Montreal, Canada, 2022-08-15 - 2022-08-19. (LA-UR-22-27890)

Heneghan, J. P., B. D. Newman, E. R. Moore, K. R. Carter, S. D. Ware, A. D. Collins, D. Musa and S. A. Sevanto. Simulating Hydrologic Field Conditions in a Greenhouse Setting for Agricultural Experiments. Presented at *International Symposium on Climate-Resilient Agri-Environmental Systems*, Dublin, Ireland, 2022-06-07 - 2022-06-10. (LA-UR-22-20789)

Heneghan, J. P., B. D. Newman, E. R. Moore, S. D. Ware, D. Musa, K. R. Carter, A. D. Collins and S. A. Sevanto. simulating Hydrologic Field Conditions in a Greenhouse Setting. Presented at *AGU Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31953)

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Other

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Carter, K. R., C. M. Yeager, E. R. Moore, L. T. Dickman, E. A. Gomez, E. M. Rodriguez, J. P. Heneghan, B. D. Newman, R. J. Harris, O. C. Marina, A. C. Nachtsheim, G. B. Perkins, C. R. Steadman and S. A. Sevanto. Drought and microbiome influence soil and root exudate chemistry. Dataset. (LA-UR-23-21050)

Carter, K. R., C. M. Yeager, E. R. Moore, L. T. Dickman, E. A. Gomez, E. M. Rodriguez, J. P. Heneghan, B. D. Newman, R. J. Harris, O. C. Marina, A. C. Nachtsheim, G. B. Perkins, C. R. Steadman and S. A. Sevanto. Root morphology influences exudates in a drought and microbiome experiment. Dataset. (LA-UR-23-21051)

Carter, K. R., C. M. Yeager, E. R. Moore, L. T. Dickman, E. A. Gomez, E. M. Rodriguez, J. P. Heneghan, B. D. Newman, R. J. Harris, O. C. Marina, A. C. Nachtsheim, B. D. Perkins, C. R. Steadman and S. A. Sevanto. Drought and microbiome influence plant physiology. Dataset. (LA-UR-23-21066)

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Kim, N. E. Lubbers, J. M. Mitchell and C. M. Yeager. Directed evolution of a soil microbiome alters plant and soil drought traits. Dataset. (LA-UR-23-21067)

Mitchell, J. M. Training and Testing Data for EI_MS_ML. Dataset. (LA-UR-22-28947)

Mitchell, J. M. Effects of Microbiome and Watering Treatments on Root and Exudate Metabolomes. Dataset. (LA-UR-22-29350)

Mitchell, J. M., J. P. Heneghan and B. D. Newman. Nylon Wicks Alter Pot Chemical Gradients. Dataset. (LA-UR-22-28859)

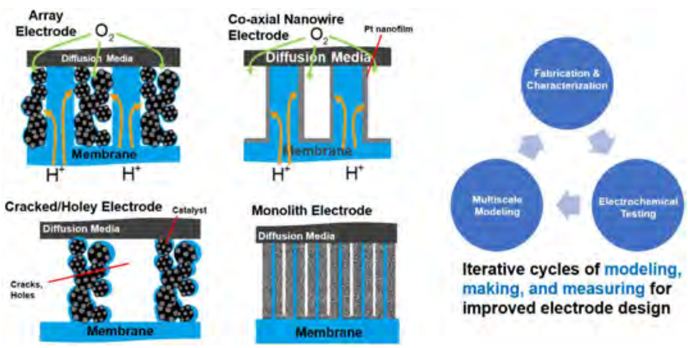
Mitchell, J. M. and S. A. Sevanto. GCxGC-TOFMS-based Metabolomics Demonstrate the Effect of the Directed Evolution of the Soil Microbiome on Maize Drought Tolerance. Dataset. (LA-UR-22-29581)

Sevanto, S. A. Stomatal closure point and plant gas exchange data from USDA Akron field experiment. Dataset. (LA-UR-21-31369)

**Peer-reviewed*

Structured Electrodes for Energy Conversion, Energy Storage, and Ionic Separations

Jacob Spendelow
20200200DR



This project focuses on design of novel electrode concepts that can provide improved performance and durability in fuel cells and other electrochemical applications. The project is developing multiple electrode concepts using a closely integrated experimental and computational approach.

Project Description

The project will address challenges associated with clean renewable energy applications and National Nuclear Security Administration (NNSA) power applications, as well as ionic separations relevant to nuclear materials. By designing improved fuel cell electrodes, we will enable substantial performance improvement and cost reduction, making clean fuel cell vehicles economically viable and increasing American competitiveness in this large and growing market. Improved fuel cell electrodes tailored specifically to NNSA fuel cell applications will also improve the ability of fuel cells to provide power generation solutions, and enable entirely new NNSA applications for fuel cells in extreme environmental conditions. Structured electrodes developed in this project will also enable less expensive and less hazardous processing of used nuclear fuel, as well as improved ionic separations and sensing for forensic and treaty verification applications.

Technical Outcomes

The project team sought to develop fundamental understanding of transport and reaction in porous electrodes, and use this understanding to develop improved electrodes for fuel cells and related applications. The team successfully developed several novel classes of electrodes, and demonstrated record-breaking performance and durability. These accomplishments were supported by extensive modeling and simulation work. The project developed and enhanced Los Alamos capabilities in microfabrication, electrochemistry, and atomistic and multiphysics modeling.

Publications

Journal Articles

Hafiz, H. and E. F. Holby. Oxygen and proton transport in flooded graphene pores with N-dopants and defects. Submitted to *Journal of Physical Chemistry C*. (LA-UR-22-21232)

Karim, M. R., T. Ahmed, W. J. de Melo Kort-Kamp, S. Komini Babu, J. S. Spendelow, E. F. Holby, M. A. Rahman and P. Chuang. Reduced-order model to optimize geometrical and structural effects on the performance of fuel cell cathodes. Submitted to *ACS Applied Energy Materials*. (LA-UR-20-29038)

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*Kim, D., T. Ahmed, K. Crossley, J. K. Baldwin, S. H. R. Shin, Y. Kim, C. Sheehan, N. Li, D. V. Pete, H. H. Han and J. Yoo. A controlled nucleation and growth of Si nanowires by using a TiN diffusion barrier layer for lithium-ion batteries. 2022. *Nanoscale Advances*. **4** (8): 1962-1969. (LA-UR-19-20571 DOI: 10.1039/D1NA00844G)

Lee, C. H., X. Wang, J. Peng, A. Katzenberg, R. K. Ahluwalia, A. Kusoglu, S. Komini Babu, J. S. Spendelow, R. Mukundan and R. L. Borup. Towards a Comprehensive Understanding of Cation Effects in Proton Exchange Membrane Fuel Cells. Submitted to *Joule*. (LA-UR-22-22836)

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Lee, C., X. Wang, J. Peng, A. Katzenberg, R. Ahluwalia, A. Kusoglu, S. Komini Babu, J. S. Spendelow, R. Mukundan and R. L. Borup. Supporting Information: Toward a Comprehensive Understanding of Cation Effects in Proton Exchange Membrane Fuel Cells. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-22-27789)

Nichols, A. W., E. N. Cook, Y. J. Gan, P. R. Miedaner, D. A. Dickie, H. S. Shafaat and C. W. Machan. Pendent Relay Enhances H2O2 Selectivity during Dioxygen Reduction Mediated by Bipyridine-Based Co–N2O2 Complexes. 2021. *Journal of the American Chemical Society*. **143** (33): 13065-13073. (LA-UR-21-27223 DOI: 10.1021/jacs.1c03381)

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Sarak, M., W. J. de Melo Kort-Kamp, F. Mojica, S. Mehrazi, M. A. Rahman and P. A. Chuang. Experimental and Computational Study on the Effeectsof Low GDL Wet proofing and Microporous Layer on PEMFC Performance. Submitted to *Energy Conversion and Management*. (LA-UR-20-26701)

Yang, G., C. H. Lee, X. Qiao, S. Komini Babu, U. Martinez and J. S. Spendelow. Advanced Electrode Structures for Proton Exchange Membrane Fuel Cells: Current Status and Path Forward. Submitted to *Advanced Materials*. (LA-UR-22-23045)

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A. Arman, M. T., A. Udiin, S. Ding, Y. He, F. Cetinbas, J. Peng, X. Wang, R. Ahluwalia, H. Xu, G. Wu, S. Komini Babu, S. Litster, U. Pasaogullari and J. S. Spendelow. Patterned Nafion Membranes for Improved Transport in PGM-free PEMFC Cathodes. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-08 - 2022-10-13. (LA-UR-22-30560)

Komini Babu, S., J. S. Spendelow, R. Mukundan, R. L. Borup and M. T. A. Arman. Cation Transport in Fuel Cell: Understanding and Suppression. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Alabama, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30335)

Komini Babu, S., M. T. A. Arman and J. S. Spendelow. Patterned Nafion Membranes for Improved Transportin PGM-free PEMFC Cathodes. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30561)

Gupta, A. J. Materials and Interfaces for Electrocatalytic Hydrogen Production and Utilization. . (LA-UR-21-21917)

Hafiz, H. and E. F. Holby. Atomistic modeling of transport for fuel cell structured electrodes. . (LA-UR-21-23835)

Holby, E. F. w22_electrocat Scientific Highlight. . (LA-UR-23-23064)

Holby, E. F. and H. Hafiz. w21_transportmd Scientific Highlight (Hafiz). . (LA-UR-22-24866)

Ince, A. C., M. F. Serincan, E. F. Holby, U. Pasaogullari, J. S. Spendelow and W. J. de Melo Kort-Kamp. Triple-Phase Pore Network for Oxygen and Proton Transport Model in the Cathode Catalyst Layer of Proton Exchange Membrane Fuel Cells. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-14. (LA-UR-22-30439)

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R. Liyanage, W. P., G. Yang, S. Komini Babu and J. S. Spendelow. Polymer Electrolyte Fuel Cell Electrodes with Improved Durability. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30364)

R. Liyanage, W. P., S. Komini Babu and J. S. Spendelow. Thin Film Catalysts Architecture for Polymer Electrolyte Fuel Cells. Presented at *Gordon Research Conference (GRC) - Fuel Cells*, Smithfield, Rhode Island, United States, 2022-07-24 - 2022-07-29. (LA-UR-22-26840)

Martinez, U., S. Komini Babu, J. S. Spendelow, R. L. Borup and A. J. Gupta. Hydrogen Energy: Production and Utilization for a Green Economy. . (LA-UR-20-26906)

Mukundan, R., R. L. Borup, E. J. Park, S. Komini Babu, J. S. Spendelow and S. Maurya. LANL Fuel Cell Program Overview. . (LA-UR-22-24954)

Osmieri, L., M. T. A. Arman, G. Wang, H. Wang, S. Komini Babu, K. C. Neyerlin and J. S. Spendelow. Electrochemical Diagnostics and Innovative Electrode Architectures to Investigate and Improve Mass Transport in Platinum Group Metal-Free Catalyst Layers. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30092)

Rahman, M. A. Structured Electrodes for PEM Fuel Cells. Presented at *Thermal and Electrochemical Energy Laboratory, University of California, Merced*, Merced, California, United States, 2020-06-04 - 2020-06-04. (LA-UR-20-24034)

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Spendelow, J. S. Fuel Cell Membrane Electrode Assemblies. Presented at *Disruptech*, Los Alamos, New Mexico, United States, 2021-02-24 - 2021-02-26. (LA-UR-21-21545)

Spendelow, J. S. Fuel Cell Membrane Electrode Assemblies. Presented at *DisrupTECH*, Los Alamos, New Mexico, United States, 2021-08-18 - 2021-08-18. (LA-UR-21-28129)

Spendelow, J. S. Structured Electrodes for Energy Conversion, Energy Storage, and Ionic Separations. . (LA-UR-22-25298)

Posters

Komini Babu, S., M. T. A. Arman, J. S. Spendelow, R. Mukundan and R. L. Borup. Understanding and Suppression of Cation Transport into Polymer Electrolyte Membrane Fuel Cell. Presented at *M2FCT meeting*, Napa, California, United States, 2022-08-30 - 2022-09-01. (LA-UR-22-28901)

**Peer-reviewed*

Electrochemical Carbon Dioxide (CO2) Conversion: Towards Higher Energy-Density Chemicals

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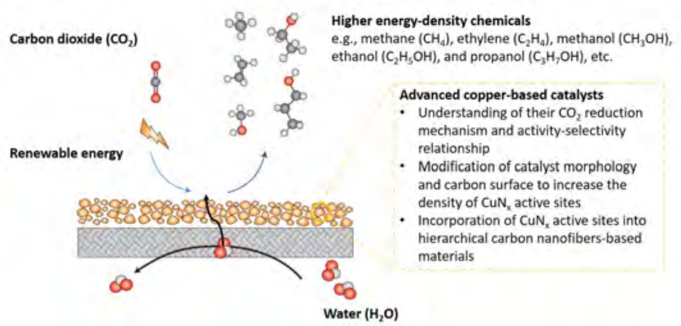
20220673DR



Researchers at Los Alamos National Laboratory are developing novel strategies for designing advanced copper-based electrocatalysts to synthesize high energy-density fuels through electrochemical CO2 conversion, reduce carbon pollution and mitigate dependence on fossil fuels.

Project Description

This project addresses the important national security challenge on climate impacts and energy security through eletrochemical conversion of Carbon Dioxide (CO2) to high energy-density fuels using electricity from renewable sources. The challenge of this technology comes from competing with hydrogen evolution reaction and low selectivity for the desirable multicarbon products. The key to solve this problem relies on precisely engineering materials properties for selective reduction of CO2 molecules towards desired products. To address this challenge, the proposed work will focus on understanding of Carbon Dioxide reduction reaction (CO2RR) mechanism and role of atomically dispersed copper coordinated by x nitrogen atom (CuNx) sites in copper-nitrogen-carbon (Cu-N-C) catalysts, modification of catalyst morphology and carbon surface to increase the active site density, and functionalization of hierarchical carbon nanofibers with CuNx sites to obtain high-performance copper-based catalysts for CO2RR. Successful demonstration of electrochemical conversion technology will result in meaningful portfolio, subsequently drawing industrial interest. Such an interest will ultimately lead to either collaborative or work-for-others projects funded by the private sector.

Technical Outcomes

This project has successfully synthesized copper (Cu) aerogel electrocatalysts for carbon dioxide reduction, with higher surface area (up to 132 m2/g) and larger pore volumes (up to 2.3 cm3/g) compared to Cu nanoparticle catalysts. In electrochemical testing, high meso- and macroporosities of aerogels have been found to benefit mass-transport properties and activity of catalysts. The safe upper potential limit for Cu catalysts has determined to be 0.65 V versus reversible hydrogen electrode.

Publications

Presentation Slides

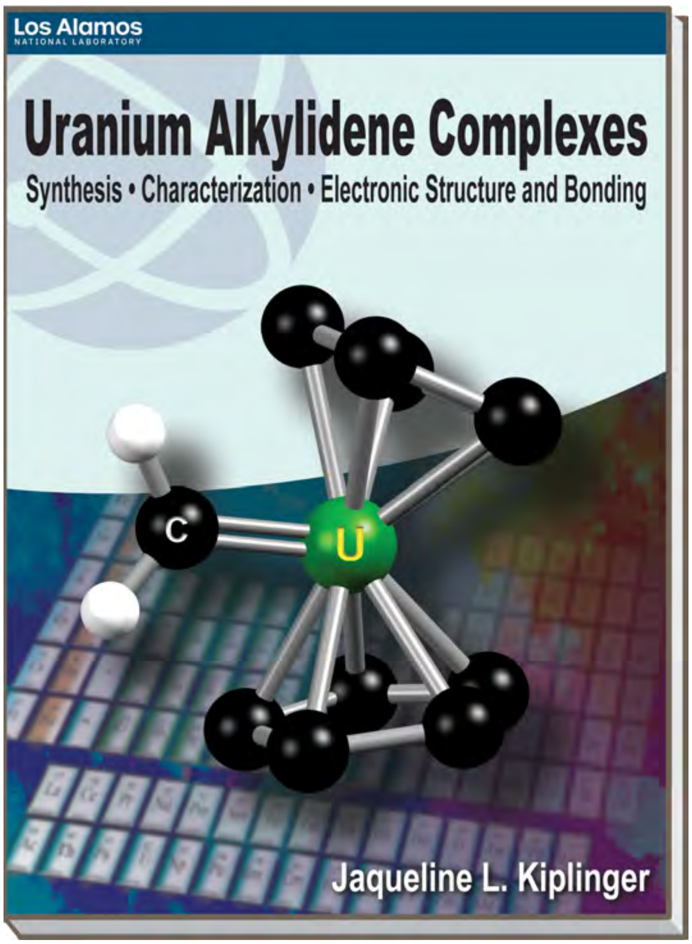
He, Y., J. C. Weiss, J. D. Jernigen and P. Zelenay. Me-N-C Electrocatalysts for Electrochemical CO2 Reduction to High-Value Products. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30428)

He, Y., J. C. Weiss and P. Zelenay. Effect of Nanostructure and Surface Chemistry on Activity and Selectivity of Cu-Based Electrocatalysts for Carbon Dioxide Reduction. Presented at *Electrochemical Society (ECS) Spring Meeting*, Vancouver, Canada, 2022-05-29 - 2022-06-02. (LA-UR-22-24965)

**Peer-reviewed*

Capturing the First Uranium Alkylidene Complex

Jaqueline Kiplinger
20200338ER



The figure displays a textbook featuring the first molecular uranium alkylidene complex, a compound that contains a U=C double bond. These compounds, which have eluded the chemistry community for over 50 years, could be the key to understanding a variety of gas forming reactions mediated by actinide metals. Actinide chemistry and LDRD researcher, Jaqueline Kiplinger, and her team have combined synthesis, experiment, and theory to advance our understanding of these enigmatic compounds. [Image credit: Josh Smith, Chemistry Division Office]

Project Description

Los Alamos has positioned itself as an institute of excellence at the forefront of actinide science. This proposal will deliver the first isolable uranium alkylidene complex, which is a molecule that contains a covalent uranium carbene (U=C) double bond. Actinide alkylidene complexes have eluded the community as a whole despite intense interest and the pursuit of many synthetic avenues. With the isolation of a uranium alkylidene complex, spectroscopy and theoretical calculations will be used to better understand the participation of flouride ion electrons and orbitals in its bonding and chemistry. The link between transition-metal alkylidenes and the degradation of hydrocarbons in plastics and rubbers is intriguing since it stands to reason that actinide analogues could react in a similar fashion. In light of the Waste Isolation Pilot Plant (WIPP) incident and the evolution of reactive gas mixtures from actinide waste storage tanks at the Hanford Site, understanding the range of reactions that are mediated by actinide alkylidenes should provide insight into potential waste storage/compatibility issues.

Publications

Journal Articles

Ramirez, B. L., E. Nicolas, B. L. Scott, D. E. Morris, T. Cantat and J. L. Kiplinger. Reductive Cleavage of Sigma Bonds by Thorium(IV) Complexes Containing Redox-Active Arene Ligands. Submitted to *Journal of the American Chemical Society*. (LA-UR-23-22636)

Presentation Slides

Garcia, N. A., B. L. Ramirez, J. L. Kiplinger and C. Lu . Synthesis, Characterization, and Reactivity of a New Class of Uranium Complexes Supported by Nitrogen/Phosphorus Ligands. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-28556)

Ramirez, B. L. Reductive Cleavage of Sigma Bonds by Thorium(IV) Complexes Containing Redox-Active Arene Ligands. Presented at *Seaborg Actinide Lecture Series*, Los Alamos, New Mexico, United States, 2023-02-08 - 2023-02-08. (LA-UR-23-20972)

Ramirez, B. L., E. Nicolas, B. L. Scott, D. E. Morris, T. Cantat and J. L. Kiplinger. Reductive Cleavage of Sigma Bonds by Thorium(IV) Complexes Containing Redox-Active Arene Ligands. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, Indianapolis, Indiana, United States, 2023-03-26 - 2023-03-30. (LA-UR-23-22934)

**Peer-reviewed*

Infiltrating the Epigenetic Code: Identifying 3-Dimensional Chromosome Signatures of Viral Infection

Karissa Sanbonmatsu
20210134ER

This work involves simulations large-scale conformational changes of a chromosome with simultaneous evolution of epigenetic marks and RNA binding, based on Hi-C data. Creation of RNA and protein particles was simulated, along with their diffusion through and around the chromosome. The project team used these simulations to emulate ternary complex formation of RNA, chromatin and polycomb repressive complex 2, spreading of epigenetic marks and RNA binding across the chromosome, as observed experimentally in cell biology experiments.

Project Description

Chromosomes play a key role throughout biomedicine and biomedical-related issues, including viral infections, cancer, brain function and childhood development. Despite this importance, little is known about how exactly chromosomes work. In particular, many scientists believe that the shape of the chromosome directly influences its working processes (function); however, the direct evidence to prove this is lacking. We will use state-of-the-art supercomputers and algorithms in combination with new experimental biology techniques to examine the relationship between the shape of the chromosome and the things that the chromosome does.

Publications

Journal Articles

Lappala, A., C. Y. Wang, A. Kriz, H. M. Michalk, K. Tan, J. Lee and K. Y. Sanbonmatsu. 4D chromosome reconstruction elucidates the spatial reorganization of the mammalian X-chromosome. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-21-29486)

Books/Chapters

Steadman, C. R. Chapter 17: Epigenetics in Algae. (LA-UR-21-32100)

Presentation Slides

Venu, V., S. Banerjee, C. K. Sanders, A. J. Sabella, B. L. Marrone, S. N. Twary and C. R. Steadman. Deciphering the role of DNA methylation in lipid accumulation in Tetraselmis Striata. Presented at *SMBE Global symposia 9, 2023-02-28/2023-03-01 (Online, New Mexico, United States)*, Online, New Mexico, United States, 2023-02-28 - 2023-02-28. (LA-UR-23-22029)

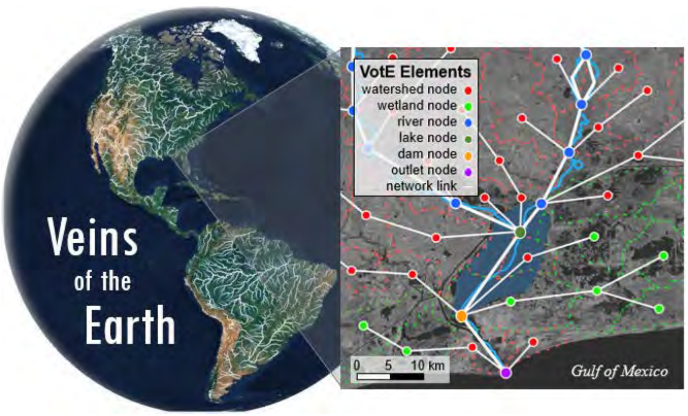
Posters

Venu, V., C. J. N. Roth, S. N. Micheva-Viteva, S. H. Adikari, K. Y. Sanbonmatsu, S. R. Starkenburg and C. R. Steadman. Understanding the interplay between histone modifications and chromatin configuration in the human genome. Presented at *Cold Spring Harbor Conference : Genome organization and nuclear function*, Cold Spring Harbor, New York, United States, 2022-05-03 - 2022-05-07. (LA-UR-22-23778)

**Peer-reviewed*

A Global, High-Resolution River Network Model for Improved Flood Risk Prediction

Jonathan Schwenk
20210213ER



Veins of the Earth (VotE) captures the many ways in which water moves across the Earth's surface, from watersheds to rivers and reservoirs and ultimately lakes and oceans. Each component that affects how water travels through the network is represented as an object in a graph, giving VotE vast flexibility to modifications and leading to efficient flow-routing simulations. VotE can be driven with Earth System Models to answer questions about flood risk projections at global scales, but has the precision to also answer questions at local scales, such as "What happens to water flow if we place a dam here?"

Project Description

Floods continue to be the most destructive natural disaster worldwide (~$20 billion in infrastructure damages and 2 million human displacements) despite significant research effort and money aimed at predicting and mitigating hazards. Our work aims to provide a new baseline for monitoring and modeling both flooding and water resources generally. This work will minimize the uncertainty surrounding flood projections by creating a high-resolution, vector-based representation of global river networks made possible by the ever-growing archives of remotely-sensed data. This supports the Department of Energy (DOE) mission, which invested significantly in the Energy Exascale Earth System Model (E3SM) that has seen only limited use for flood projections due largely to uncertainties in runoff prediction. Our work will directly address this challenge by minimizing flow-routing uncertainties, which in turn enables improved diagnosis for errors in runoff projections. Our state-of-the-art model of the "veins of the Earth" has additional relevance to a number of DOE challenges including water security, water infrastructure, and hydroelectric power generation. Our focus on the global river network will go beyond the Earth System Models (including Energy Exascale Earth System Model or E3SM) by establishing an efficient mechanism for answering questions about water security dynamics under possible climate scenarios.

Publications

Journal Articles

*Boero, R., C. J. Talsma, J. A. Oliveto and K. E. Bennett. Expectations of Future Natural Hazards in Human Adaptation to Concurrent Extreme Events in the Colorado River Basin. 2022. *Climate*. **10** (2): 27. (LA-UR-20-28365 DOI: 10.3390/cli10020027)

Chen, B., K. Miller, A. Bertozzi and J. P. Schwenk. Graph-based Active Learning for Surface Water and Sediment Detection in Multispectral Images. Submitted to *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-22-28645)

Chen, B., K. Miller, A. Bertozzi and J. P. Schwenk. Batch active learning for multispectral and hyperspectral image segmentation using similarity graphs. Submitted to *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*. (LA-UR-22-32206)

Chen, B., K. Miller, A. Bertozzi and J. P. Schwenk. Graph-based Active Learning for Surface Water and Sediment Detection. Submitted to *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*. (LA-UR-23-20513)

*Hariharan, J., A. Piliouras, J. Schwenk and P. Passalacqua. Width-Based Discharge Partitioning in Distributary Networks: How Right We Are. 2022. *Geophysical Research Letters*. **49** (14): e2022GL097897. (LA-UR-22-24645 DOI: 10.1029/2022GL097897)

Knights, D., A. Piliouras, J. P. Schwenk, J. Hariharan and C. Russoniello. Seasonal and Morphological Controls on Nitrate Retention in Arctic Deltas. Submitted to *Geophysical Research Letters*. (LA-UR-22-32180)

Schwenk, J. P., T. Zussman, J. C. Rowland and J. J. Stachelek. rabpro: global watershed boundaries, river elevation profiles, and catchment statistics. 2022. *Journal of Open Source Software*. **7** (73): 4237. (LA-UR-22-22609 DOI: 10.21105/joss.04237)

Schwenk, J. P. and J. Hariharam. RivGraph: Automatic extraction and analysis of river and delta channel network topology. 2021. *Journal of Open Source Software*. **6** (59): 2952. (LA-UR-21-20218 DOI: 10.21105/joss.02952)

Stachelek, J. Quantifying uncertainty in Pareto estimates of global lake area. Submitted to *Limnology and Oceanography: Methods*. (LA-UR-21-30122)

Stachelek, J., P. J. Hanly and P. A. Soranno. Imperfect slope measurements drive overestimation in geometric cone model of lake and reservoir depth. Submitted to *Inland Waters*. (LA-UR-21-31329)

*Talsma, C. J., K. E. Bennett and V. V. Vesselinov. Characterizing Drought Behavior in the Colorado River Basin Using Unsupervised Machine Learning. 2022. *Earth and Space Science*. **9** (5): e2021EA002086. (LA-UR-20-28366 DOI: 10.1029/2021EA002086)

*Wagner, A. M., K. E. Bennett, G. E. Liston, C. A. Hiemstra and D. Cooley. Multiple Indicators of Extreme Changes in Snow-Dominated Streamflow Regimes, Yakima River Basin Region, USA. 2021. *Water*. **13** (19): 2608. (LA-UR-21-29336 DOI: 10.3390/w13192608)

Reports

Schwenk, J. P. and C. X. Ren. A new era of observationally-infused E3SM: GANs for unifying imagery archives. Unpublished report. (LA-UR-21-21852)

Presentation Slides

Bennett, K. E. Hydroclimate extremes in the Colorado River Basin. Presented at *Watershed Science Community Call*, Online, New Mexico, United States, 2021-11-09 - 2021-11-09. (LA-UR-22-20659)

Ranasinghe, N. R. Application of scientific machine learning to geosciences. . (LA-UR-23-21904)

Schwenk, J. P. A Platform for the Next Generation of Data-driven, River- and Watershed-centric Modeling: Veins of the Earth. Presented at *Tri Lab Climate Workshop*, Albuquerque, New Mexico, United States, 2022-12-07 - 2022-12-08. (LA-UR-22-32696)

Schwenk, J. P., J. Stachelek, J. C. Rowland, K. E. Bennett, E. M. Prior and T. Zussman. A Platform for the Next Generation of Data-driven, River and Watershed-centric Modeling: Veins of the Earth. Presented at *University of California Irvine Civil Engineering Departmental Seminar Series*, Irvine, California, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-24093)

Schwenk, J. P., J. Stachelek, K. E. Bennett, J. C. Rowland, T. Zussman and E. M. Prior. A fusion of global-scale, river-centric datasets for rapid analysis and modeling frameworks: Veins of the Earth. Presented at *USGS Community for Data Integration Geomorphology Focus Group Meeting*, Urbana, Illinois, United States, 2021-10-26 - 2021-10-26. (LA-UR-21-30613)

Schwenk, J. P. and J. Hariharan. Exploring river and delta channel networks with RivGraph. Presented at *Community Surface Dynamics Modeling System Annual Meeting*, Boulder, Colorado, United States, 2021-05-20 - 2021-05-20. (LA-UR-21-30437)

Posters

Stachelek, J., J. P. Schwenk and K. E. Bennett. Flexible Integration of Lakes in Global River Systems. Presented at *American Geophysical Union (AGU) Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-32058)

Other

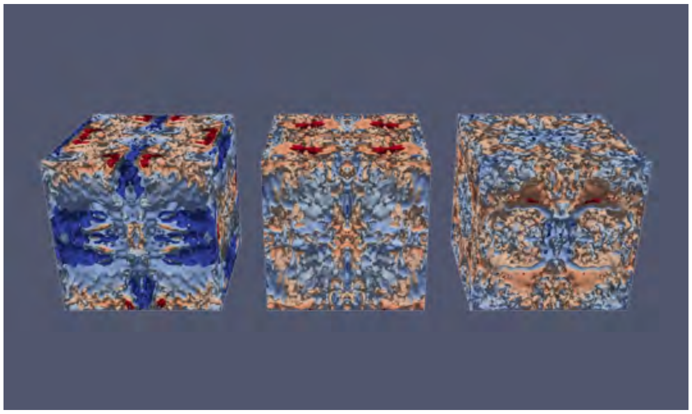
Bennett, K. E., C. Talsma, J. Stachelek and J. P. Schwenk. Historical and Future Extreme Event Indices for the Colorado River Basin.. Dataset. (LA-UR-22-22746)

Schwenk, J. P., J. C. Rowland and E. M. Prior. Creating a Global Dam Dataset for River Network Integration. Dataset. (LA-UR-21-28088)

**Peer-reviewed*

Local Transition Modeling for Mixing

Daniel Israel
20210218ER



The mixing of materials can depend strongly upon the details of their initial configuration at small scales. Here, researchers from Los Alamos use direct numerical simulation to examine how different initial conditions effect the statistics and morphology of the mixture at later times. This information is important for creating new, advanced models for transition and turbulence.

Project Description

Laminar-turbulent transition is the process by which the flow of a fluid goes from smooth and predictable to complex and unpredictable. It can be observed in the flow from a sink faucet, changing from glassy to frothy as the flow rate is increased. Predicting transition is critical to predicting the flow, and our current models are insufficient to the simulation challenges we face. Addressing this challenge is important for our predictive capabilities for nuclear weapons and will impact National Nuclear Security Administration (NNSA) key mission priorities of stockpile stewardship, nuclear forensics, and non-proliferation.

Publications

Journal Articles

Bhattacharya, A., D. M. Israel and R. W. Robey. Accelerating Python-based platform portable DNS using MPI on GPU architectures. Submitted to *TBD*. (LA-UR-22-29282)

Israel, D. M. The Boussinesq Approximation Applied to Variable Density Flow. Submitted to *Physical Review Fluids*. (LA-UR-22-23308)

Conference Papers

Israel, D. M., K. A. Flippo and F. W. Doss. Transition Modeling at Los Alamos National Laboratory. Presented at *AIAA Aviation and Aeronautics Forum and Exposition*. (Chicago, Illinois, United States, 2022-06-27 - 2022-07-01). (LA-UR-22-23994)

Presentation Slides

Israel, D. M. Transition Modeling for the Taylor-Green Vortex. Presented at *73rd Annual Meeting of the APS Division of Fluid Dynamics*, Online, New Mexico, United States, 2020-11-22 - 2020-11-24. (LA-UR-20-29647)

Israel, D. M. Linear Stability Analysis of the RANS Equations for Transition. Presented at *LANL Arizona Days*, Los Alamos, New Mexico, United States, 2022-08-15 - 2022-08-16. (LA-UR-22-29419)

Israel, D. M., K. A. Flippo and F. W. Doss. Transition Modeling at Los Alamos National Laboratory. Presented at *AIAA Aviation and Aeronautics Forum and Exposition*, Chicago, Illinois, United States, 2022-06-27 - 2022-07-01. (LA-UR-22-23995)

Israel, D. M., K. A. Flippo and F. W. Doss. Transition Modeling at Los Alamos National Laboratory. Presented at *AIAA Aviation and Aeronautics Forum and Exposition*, Chicago, Illinois, United States, 2022-06-27 - 2022-07-01. (LA-UR-22-24257)

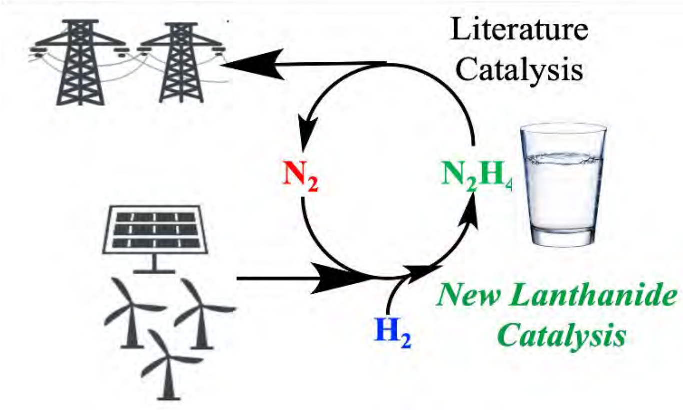
Israel, D. M. and A. P. Haas. Local Transition Modeling for Mixing: Year 2 LDRD-ER Review. . (LA-UR-22-33031)

Safarik, I. L. and A. Bhattacharya. Parallelization of Python DNS Code. . (LA-UR-22-27653)

**Peer-reviewed*

Grid Scale Energy Storage Using Hydrazine Produced from Lanthanide Electrocatalysis

Benjamin Davis
20210251ER



The demand for grid-scale energy storage has shifted to longer time-scales and as result sponsors are looking for new paradigms involving liquid materials. Using an electrocatalytic approach, we will develop lanthanide catalysts that convert dinitrogen and renewably produced hydrogen into the energy rich liquid hydrazine (N2H4). When there is energy demand on the grid, known literature catalysts can transform N2H4 back to hydrogen (H2) which will be converted to electricity using proton-exchange membrane fuel cells.

Project Description

To facilitate greater renewable energy utilization and resiliency of our electrical grid, energy storage has been the focus of several offices within the Department of Energy. The Office of Electricity & Renewable Energy (EERE) and the Advanced Research Projects Agency - Energy (ARPA-e) are both targeting energy-rich materials for storage. We aim to study the fundamental chemical reactions necessary to make one such material, hydrazine, using hydrogen and dinitrogen gas - the same components used to make ammonia on a massive scale industrially. By combining lanthanide complexes reported in the literature, along with our expertise in modeling and synthesis, we believe we can develop an electrocatalytic cycle to make hydrazine efficiently. The combination of our cycle with known methods to convert hydrazine into electricity could establish a new paradigm to store energy on the grid-scale - addressing our national need.

Publications

Journal Articles

*McNeece, A. J., A. Jaros, E. R. Batista, P. Yang, B. L. Scott and B. L. Davis. Hydrazine Energy Storage: Displacing N2H4 from the Metal Coordination Sphere. 2022. *ChemSusChem*. **15** (18): e202200840. (LA-UR-22-26735 DOI: 10.1002/cssc.202200840)

Yuan, M. Application of Computational Methods to Unraveling the Mechanism and Reactivity of Metallaphotoredox Dual Catalysis. Submitted to *Chem*. (LA-UR-22-32845)

Reports

Yuan, M., P. Yang and E. R. Batista. Current Progress on the Mechanistic Exploration and Spectroscopic Study of Lutetium Dinitrogen Complex. Unpublished report. (LA-UR-22-31777)

Presentation Slides

Davis, B. L., A. J. McNeece, E. Dolgopolova and L. E. Wolfsberg. Unusual Photochromic Behavior in Lutetium Dinitrogen Complexes. Presented at *American Chemistry Society National Meeting*, Indianapolis, Indiana, United States, 2023-03-30 - 2023-03-30. (LA-UR-23-23106)

McNeece, A. J., B. L. Davis, P. Yang, E. R. Batista and A. Jaros. Lanthanide Catalysts for Direct Conversion of N2 to N2H4. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, San Diego, California, United States, 2022-03-20 - 2022-03-24. (LA-UR-22-22648)

McNeece, A. J. and B. L. Davis. Lanthanide Catalysts for Direct Conversion of N2 to N2H4. Presented at *Fall ACS Conference*, Atlanta, Georgia, United States, 2021-08-26 - 2021-08-26. (LA-UR-21-28436)

Posters

Yuan, M., B. L. Davis, E. R. Batista and P. Yang. Competition in the Bonding Interactions of N2 with 4f Element. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21763)

Other

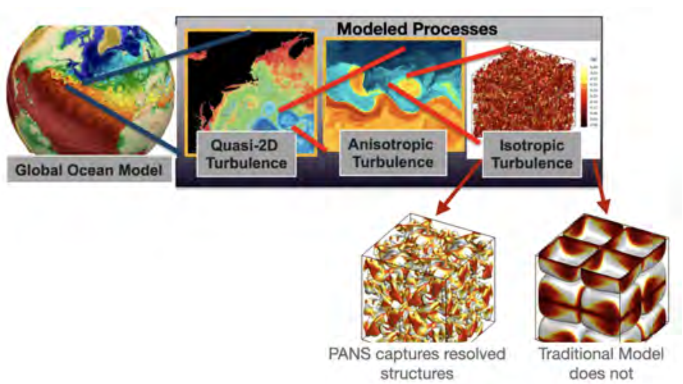
Popov, I. A. Dataset of Density Functional Theory (DFT) Calculations on Redox Flow Batteries and Transition Metal/Lanthanide/Actinide Containing Complexes. Dataset. (LA-UR-21-26186)

**Peer-reviewed*

Blurring the Lines Between Ocean Parameterization and Large Eddy Simulation

Luke Van Roekel

20210289ER



Oceanic flows contain a multitude of time and spatial scales that must be modeled. Current models exist for each scale of motion separately. Researchers at LANL, through the support of LDRD funding, are developing a new class of models that can span scales, modeling specified structures. This technique; Partially Averaged Navier Stokes (PANS) has been applied in a number of idealized flows (bottom), but has never before been applied to oceanic flows.

Project Description

The primary goal of this research is a new ocean model that accurately and efficiently simulates important oceanic processes across horizontal scales. Additionally the heart of this model (a new representation of turbulent flows in the ocean) will be important to not only Department of Energy (DOE) interests but also the broader earth science community. This work directly impacts the DOE Office of Science mission to achieve predictive understanding of nature to enhance energy, economic, and national security. This project will lead to advances in model projections of how the ocean will change the energy and water security of the United States. Direct impacts through storm surge and sea level rise will be improved, in turn improving information for decisions related to coastal energy infrastructure. The ocean also has a leading order impact on future sea ice distributions having dramatic national security implications (e.g. understanding when the Northwest passage may open). Our work will impact numerous DOE projects (the Energy Exascale Earth System Model) and various coastal modeling initiatives recently funded by DOE. The capabilities developed in this proposal will also place DOE at the forefront of multiresolution Earth System Modeling and modeling of small scale turbulence for the ocean.

Publications

Journal Articles

Soares Pereira, F. M., F. Grinstein, D. M. Israel and L. Eca. Verification and Validation: the Path to Predictive Scale-Resolving Simulations of Turbulence. Submitted to *Journal of Verification, Validation and Uncertainty Quantification*. (LA-UR-21-22615)

Van Roekel, L., D. Engwirda and S. Calandrini. A nonhydrostatic formulation for MPAS-Ocean. Submitted to *Geoscientific Model Development*. (LA-UR-22-25691)

Presentation Slides

Soares Pereira, F. M., D. M. Israel and L. Van Roekel. Development of Hybrid RANS/LES Model for Oceanic Turbulent Flows. Presented at *APS-DFD 2022*, Indianapolis, Indiana, United States, 2022-11-19 - 2022-11-22. (LA-UR-22-32076)

Soares Pereira, F. M., F. Grinstein, D. M. Israel and L. Eca. Verification & Validation Strategy for Scale-Resolving Simulations of Turbulence. Presented at *V&V Symposium*, (Virtual), New Mexico, United States, 2021-05-19 - 2021-05-19. (LA-UR-21-23591)

Soares Pereira, F. M., L. Eca, G. Vaz, F. Grinstein, D. M. Israel, R. M. Rauenzahn and S. Girimaji. Toward Predictive Viscous Simulations in Naval Architecture and Marine Engineering. . (LA-UR-22-21700)

Serna, J. J., D. Paeres Castano, F. M. Soares Pereira, L. Van Roekel and D. M. Israel. Global Ocean Modeling: Assessment of KPP vs. GLS Models.. Presented at *2022 CPW Poster presentation*, Los Alamos, New Mexico, United States, 2022-08-18 - 2022-08-18. (LA-UR-22-28782)

Posters

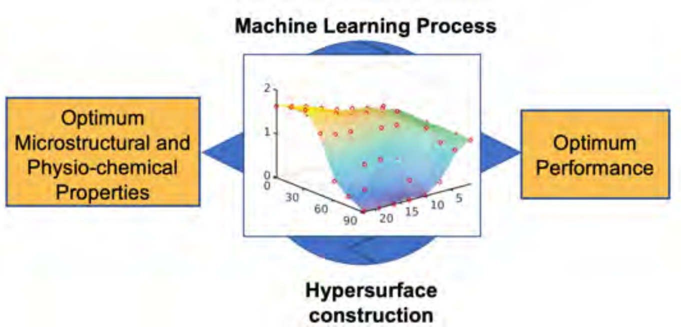
Paeres Castano, D., J. J. Serna, F. M. Soares Pereira, L. Van Roekel and D. M. Israel. Global Ocean Modelling: Assessment of KPP vs. GLS turbulence models. Presented at *2022 CPW Poster presentation*, Los Alamos, New Mexico, United States, 2022-08-18 - 2022-08-18. (LA-UR-22-28313)

Soares Pereira, F. M., D. M. Israel and L. Van Roekel. Partially-Averaged Navier-Stokes Equations Model for Prediction of Turbulent Ocean Flows. Presented at *American Mathematical Society (AMS) Meeting*, Breckenridge, Colorado, United States, 2022-06-12 - 2022-06-17. (LA-UR-22-25433)

**Peer-reviewed*

New Possibilities and Discovery Methods for Explosives Synthesis and Formulation

William Perry
20210339ER



The image shows schematically how our machine learning tool will find the relationships between microstructural and physio-chemical parameters of the explosive and its performance. Once trained, the tool will guide the designer to choose explosive characteristics that will achieve performance goals.

Project Description

Improved predictive capabilities for high explosives sensitivity and performance are critical to the national security mission. We have the potential to revolutionize high explosive science, development, discovery, surveillance, quality control and safety. Our primary goal is to pair cutting edge machine learning techniques with a newly developed, physics-aware reactive burn model to incorporate microstructural data from actual stockpile explosives and improve our predictive capabilities. Following on from this, we will use what we've learned to improve the viability of a new potential stockpile explosive and then to "design" from scratch a completely novel explosive. We will also provide a path to an engineering level methodology for these activities, which would drastically reduce time and cost for existing and new explosive evaluation and analysis, a game-changer for Department of Energy (DOE)/National Nuclear Security Administration (NNSA) programs such as current/future Life Extension Programs, the Advanced Scientific Computing program, the Joint Department of Defense (DOD)/DOE Munitions Program and Campaign 2 High Explosive Science Program. With this combined theoretical-experimental approach, we will lay the foundation for future detailed efforts which will improve the properties (safety, performance, manufacturability, etc.) of specific explosives for targeted applications.

Publications

Journal Articles

. D. A. L. *. M. J. T. *. C. D. B. Perry, W. L., A. L. Duque, J. T. Mang, D. B. Culp and W. L. Perry. Computing continuum-level explosive shock and detonation response over a wide pressure range from microstructural details. 2021. *Combustion and Flame*. **231: 111470. (LA-UR-20-30427 DOI: 10.1016/j.combustflame.2021.111470)

Perry, W. L., A. L. Duque, J. T. Mang and D. B. Culp. A physically-informed, surface area-dependent, wide pressure range continuum reactive flow model. Submitted to *Combustion and Flame*. (LA-UR-20-30125)

*Walters, D., N. Rai, O. Sen and W. L. Perry. Toward a machine-guided approach to energetic material discovery. 2022. *Journal of Applied Physics*. **131** (23): 234902. (LA-UR-21-31595 DOI: 10.1063/5.0084973)

Conference Papers

Perry, W. L., T. D. Aslam and M. J. Burns. Connecting details of heterogeneous explosive reactive wave profiles to the hydrodynamic reaction rate. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*. (anahiem, California, United States, 2022-07-11 - 2022-07-11). (LA-UR-22-31760)

Presentation Slides

Walters, D. O., L. A. Lystrom, O. Sen and W. L. Perry. A machine-guided approach to connect porosity characteristics to corner turning performance in PBX 9502. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26597)

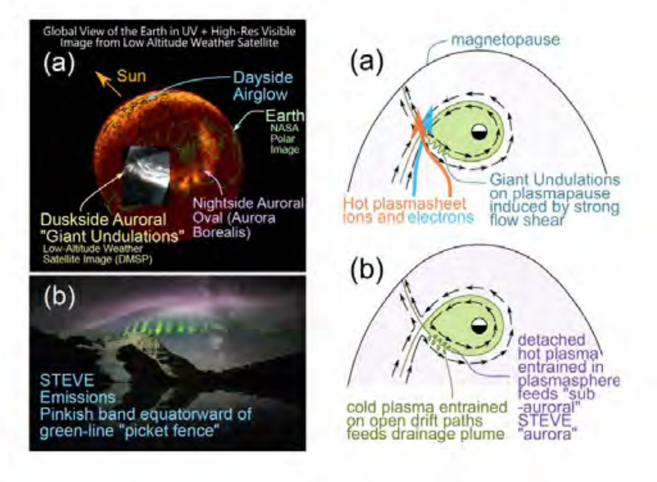
Posters

Walters, D. O., L. A. Lystrom, O. Sen and W. L. Perry. A machine-guided approach to connect porosity characteristics to corner turning performance in PBX 9502. Presented at *Gordon Research Conference (GRC) - Energetic Materials*, Manchester, New Hampshire, United States, 2022-06-26 - 2022-07-01. (LA-UR-22-25754)

**Peer-reviewed*

Cold Plasma and Plasmapause Instabilities: A Possible Driver for Long-Lived Drainage Plumes, Giant Undulations and STEVE (Strong Thermal Emission Velocity Enhancement) Aurora

Michael Henderson
20210440ER



Left a) Giant Undulation visible at the equatorward edge of the auroral distribution; Left b) Generation of sub-auroral STEVE emissions. Right a) Flow of plasmasheet particles adjacent to the dusk-side plasmasphere.; Right b) The hypothesized model; that disruption of the plasmapause boundary feeds both long-lived drainage plumes and STEVE emissions.

Project Description

The cold, dense plasma in Earth's magnetosphere plays a critical role in regulating important physics that controls the magnitude and duration of hazardous natural and man-made space weather disturbances. These include buildup and decay of Earth's ring current and radiation belts (via both solar storms and High-Altitude Nuclear Explosions (HANE)) and the overall efficiency of the solar wind/magnetosphere coupling. Understanding how these processes operate and how they impact technological systems is important for national security. Unfortunately, a detailed understanding of cold-plasma physics still eludes the space physics community. Recent work shows for the first time how cold plasma controls the amplitude of waves present in the environment and hence, its dynamics. Since current methods to clean-up space after a HANE are based on injection of plasma waves, the cold plasma is likely to be a primary factor in determining the efficiency of these schemes and a detailed understanding of its physics will provide the missing knowledge for better prediction of how these natural and man-made phenomena evolve. Los Alamos National Laboratory (LANL) is strongly invested in radiation-belt remediation and the duality between strong science and national-security applications is one of the reasons why this research must be performed at LANL.

Publications

Journal Articles

*Henderson, M. G. Key elements of auroral substorm development and their relationship to recent observations of detached sub-auroral phenomena including STEVE-like emissions. 2021. *Journal of Atmospheric and Solar-Terrestrial Physics*. 105600. (LA-UR-21-22047 DOI: 10.1016/j.jastp.2021.105600)

Henderson, M. G. Generation of STEVE-like Emissions Following Intensifications of the Poleward Boundary of the Substorm Bulge and Streamer Production. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-20-26078)

*Henderson, M. G. Association of Mesoscale Auroral Structures and Breakups With Energetic Particle Injections at Geosynchronous Orbit. 2022. *Frontiers in Astronomy and Space Sciences*. **9**: 742246. (LA-UR-21-27729 DOI: 10.3389/fspas.2022.742246)

Reports

Henderson, M. G. The Need for More Capable Space-Based Auroral Imagers. Unpublished report. (LA-UR-22-29436)

Koshkarov, O. Institutional Computing annual report for project: Global space physics simulations with reduced kinetic models. Unpublished report. (LA-UR-23-22504)

Presentation Slides

Koshkarov, O. Global simulations of instabilities in the plasmapause boundary layer. . (LA-UR-23-22510)

Yakymenko, K., V. K. Jordanova, M. A. Engel and S. K. Morley. RAM-SCB SIMULATIONS OF THE INNER MAGNETOSPHERE DURING THE CME-INDUCED GEOMAGNETIC STORM OF 6-9 SEPTEMBER 2017 AND HIGH-SPEED STREAM-DRIVEN GEOMAGNETIC STORM OF 19-26 APRIL 2017 FOR ISWAT CHALLENGE. Presented at *GEM Summer Workshop*, Honolulu, Hawaii, United States, 2022-06-19 - 2022-06-19. (LA-UR-22-25756)

Posters

Koshkarov, O., G. L. Delzanno, V. Roytershteyn and C. Pagliantini. Enabling Optimizations for Global Magnetospheric Kinetic Simulations with Reduced Kinetic Spectral Models. Presented at *AGU Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31965)

Koshkarov, O., G. L. Delzanno, V. Roytershteyn and C. Pagliantini. Enabling Optimizations for Global Magnetospheric Kinetic Simulations with Reduced Kinetic Spectral Models. Presented at *GEM Summer Workshop*, Honolulu, Hawaii, United States, 2022-06-19 - 2022-06-19. (LA-UR-22-25484)

Yakymenko, K., O. Koshkarov, G. L. Delzanno and M. G. Henderson. Numerical Studies of Plasmapause Boundary Layer Instabilities. Presented at *American Geophysical Union (AGU) Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32071)

Yakymenko, K., O. Koshkarov, G. L. Delzanno and M. G. Henderson. Numerical Studies of Plasmapause Boundary Layer Instabilities. Presented at *GEM Summer Workshop*, Honolulu, Hawaii, United States, 2022-06-19 - 2022-06-19. (LA-UR-22-25758)

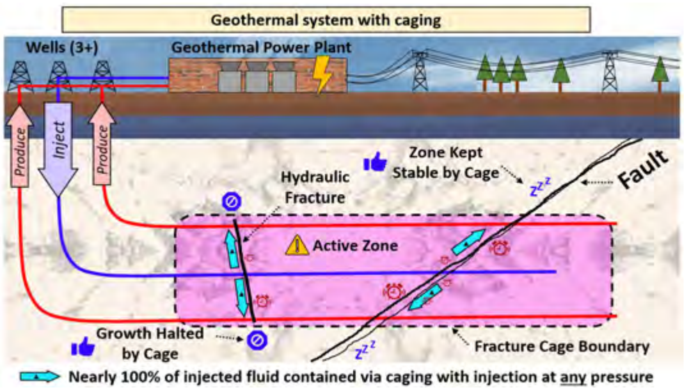
Other

Henderson, M. G. 2023 Los Alamos Space Weather Summer School Flyer. Audio/Visual. (LA-UR-22-32040)

**Peer-reviewed*

Fracture Caging: A New Method to Limit Injection-Induced Seismicity

Luke Frash
20220175ER



Fracture caging uses two or more boundary wells to capture and then produce injected fluids, thus containing the active injection zone. Caging achieves nearly 100% recovery of the injected fluid and limits the strength of earthquakes that would otherwise be triggered by fluid injection. This reduces risk and uncertainty relative to conventional approaches to enhanced geothermal systems (EGS) that rely on injection rate and pressure limits. The project team anticipates that caging will enable safe long-term high-pressure injection, increased reservoir efficiency, and improved adaptability to the uncertain and dynamic subsurface (e.g., hidden faults).

Project Description

Fracture caging could enable economic energy production from a previously unusable >60 Gigawatts (GW) of 'always-on' geothermal resources, thus providing a similar technological leap to hydraulic fracturing that brought its boom to oil & gas energy security. With 'caging', the crucial show-stopper risk of injection-induced seismicity can be readily overcome. In addition, our 'fracture caging' method will increase the efficiency of geothermal facilities while also improving the robustness of these systems amid dynamic subsurface conditions. Understanding fracture fluid flow in complex rocks supports Department of Energy/National Nuclear Security Administration missions for Applied Energy Programs (Office of Energy Efficiency and Renewable Energy, Office of Fossil Energy, and Advanced Research Projects Agency-Energy (ARPA-E)), the Civilian Nuclear Program (Used Nuclear Fuel Disposition), Basic Energy Sciences, and Nuclear Nonproliferation. Thus, it does not escape our notice that caging has significant potential beyond geothermal energy, but rising interest in clean energy technologies combined with geothermal's historic problems with injection-induced seismicity positions 'caging' to be a game changer for a clean energy future. This work will help place Los Alamos National Laboratory in a lead position in the exciting clean-green energy frontier.

Publications

Conference Papers

Ahmmed, B. and L. P. Frash. A FORGE Datathon Case Study to Optimize Well Spacing and Flow Rate for Power Generation. Presented at *Stanford Geothermal Workshop*. (Stanford, California, United States, 2023-02-06 - 2023-02-08). (LA-UR-23-20863)

Frash, L. P., J. W. Carey, B. Ahmmed, M. R. Sweeney, M. Meng, W. Li, B. K C and U. C. Iyare. A Proposal for Safe and Profitable Enhanced Geothermal Systems in Hot Dry Rock. Presented at *48th Workshop on Geothermal Reservoir Engineering*. (Stanford, California, United States, 2023-02-06 - 2023-02-08). (LA-UR-23-20959)

Frash, L. P., M. R. Sweeney, M. Meng, B. K C, U. C. Iyare, Y. Madenova, J. W. Carey and W. Li. Exploring the Limitations of Fracture Caging in NextGen Enhanced Geothermal Systems. Presented at *57th US Rock Mechanics/ Geomechanics Symposium*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-06-28). (LA-UR-23-22120)

Kneafsey, T., D. Blankenship, J. Burghardt, L. Huang, L. P. Frash and E. C. T. Team. The EGS Collab - Discoveries and Lessons from an Underground Experiment Series. Presented at *48th Workshop on Geothermal Reservoir Engineering*. (Stanford, California, United States, 2023-02-06 - 2023-02-08). (LA-UR-23-21536)

Madenova, Y., F. Suorineni and S. Xu. Automated and digitalized web tool for open stope design. Presented at *15th ISRM Congress 2023 & 72nd Geomechanics Colloquium*. (Salzburg, Austria, 2023-10-09 - 2023-10-14). (LA-UR-23-20818)

Madenova, Y., F. Suorineni and Z. Mukhamedyarova. Seismic source wave propagation analysis using laboratory AE monitoring system. Presented at *57TH US ROCK MECHANICS / GEOMECHANICS SYMPOSIUM*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-06-28). (LA-UR-23-22051)

Madenova, Y., F. Suorineni and Z. Mukhamedyarova. Effects of fractures on seismic wave propagation path: laboratory studies. Presented at *57TH US ROCK MECHANICS / GEOMECHANICS SYMPOSIUM*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-06-28). (LA-UR-23-22371)

Meng, M., L. P. Frash, B. K C, Y. Madenova, J. W. Carey and W. Li. Designing a Reliable Weak Bonded Interface for Fracture Caging Laboratory Validation. Presented at *ARMA Symposium Atlanta 2023*. (Atlanta, Georgia, United States, 2023-06-25 - 2023-03-28). (LA-UR-23-22483)

Mudunuru, M., B. Ahmmed, L. P. Frash and R. Frijhoff. Deep Learning for Modeling Enhanced Geothermal Systems. Presented at *48th Workshop on Geothermal Reservoir Engineering*. (Stanford, California, United States, 2023-02-06 - 2023-02-08). (LA-UR-23-20960)

Mudunuru, M., B. Ahmmed and L. P. Frash. Deep Learning for Modeling Enhanced Geothermal Systems. Presented at *Stanford Geothermal Workshop*. (Stanford, California, United States, 2023-02-06 - 2023-02-08). (LA-UR-23-20809)

Presentation Slides

Frash, L. P. Rock Fracture Caging to Power the Next Generation. Presented at *University of Florida - Guest speaker*, Gainesville, Florida, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-23877)

Frash, L. P. Forecasting and Controlling Injection-Induced Earthquake Maximum Magnitude. Presented at *American Rock Mechanics Association - Induced Seismicity Workshop*, Santa Fe, New Mexico, United States, 2022-06-25 - 2022-06-25. (LA-UR-22-25841)

Frash, L. P., B. K C, M. Meng, N. J. Welch, J. W. Carey and W. Li. Predicting the Unpredictable: Optimizing Geothermal Design. Presented at *CouFrac2022*, Berkeley, California, United States, 2022-11-14 - 2022-11-16. (LA-UR-22-31881)

Frash, L. P., M. Meng, W. Li, J. W. Carey and M. R. Sweeney. EGS Design Limits and Optimization using GeoDT and Caging: Case Study for EGS Collab E2/3. Presented at *US Rock Mechanics Geomechanics Symposium*, Santa Fe, New Mexico, United States, 2022-06-25 - 2022-06-29. (LA-UR-22-25843)

Other

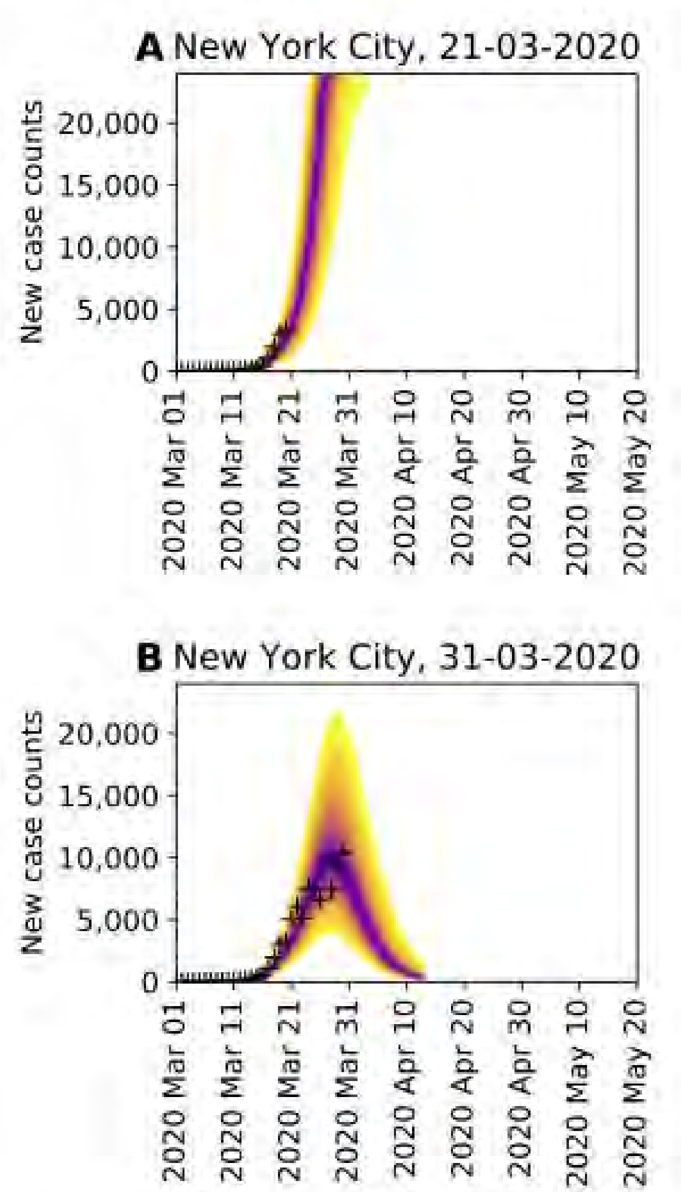
Ahmmed, B. and A. V. Noy. CEO Conversations. Audio/Visual. (LA-UR-22-33036)

Frash, L. P. FORGE_Datathon. Dataset. (LA-UR-22-25474)

**Peer-reviewed*

Modernization of Epidemiological Forecasting with Uncertainty Quantification

William Hlavacek
20220268ER



The necessity of online learning. (A) and (B) show model-based forecasts for New York City made at two different dates, as indicated. Forecasts of COVID-19 incidence up to 1 week into the future are accurate. However, forecasts must be continually updated to maintain prediction accuracy. Compare the very different predictions for 4/1 in the two plots. In each plot, the entire shaded region indicates the 95% credible interval of the predictive posterior obtained using Bayesian inference and all region-specific surveillance data available at the time of inference. The central magenta band indicates the median predicted detection of new COVID-19 cases.

Project Description

During the emergence of an infectious disease threat, the national response will be driven by expert predictions of future disease incidence, as we saw during the coronavirus (COVID-19) pandemic. Because relevant public health surveillance data will inevitably be scarce and noisy, these predictions cannot be based solely on data. Rather, mathematical models, capturing experience-informed expectations about disease transmission dynamics, must be leveraged. Generating data-driven model-based predictions, especially with quantification of prediction uncertainty, is a complex and computationally expensive task. Nevertheless, uncertainty quantification (UQ) is essential for facilitating high-stakes evidence-based decision-making. Software infrastructure currently available to support model-based epidemiological forecasting with UQ does not facilitate rapid setup of end-to-end workflows. To contribute to modernization of epidemiological forecasting infrastructure and to improve national readiness to respond to infectious disease outbreaks, we will develop an open-source community-supported software package that integrates a complete set of methods and tools needed for model-based near real-time forecasting with UQ, allowing for quick setup of forecasting jobs using best practices.

Publications

Journal Articles

Chen, Y., Y. T. Lin, E. Miller, J. Neumann, Z. He, K. Nelson, A. Mallela, R. Posner and W. S. Hlavacek. Impacts of vaccination and Severe Acute Respiratory Syndrome Coronavirus 2 variants Alpha and Delta on Coronavirus Disease 2019 transmission dynamics in the 15 most populous metropolitan statistical areas in the United States. Submitted to *Mathematical Biosciences*. (LA-UR-23-20477)

Mallela, A., Y. T. Lin and W. S. Hlavacek. Differential contagiousness of respiratory disease across the United States. Submitted to *Science*. (LA-UR-22-29514)

Miller, E. F., J. Neumann, Y. Chen, A. Mallela, Y. T. Lin, W. S. Hlavacek and R. G. Posner. Quantification of early nonpharmaceutical interventions aimed at slowing transmission of Coronavirus Disease 2019 in the Navajo Nation and surrounding states (Arizona, Colorado, New Mexico, and Utah). Submitted to *PLOS Global Public Health*. (LA-UR-23-20476)

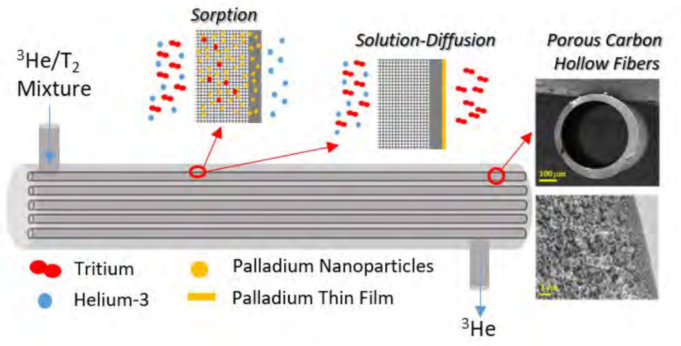
Posters

Mallela, A., J. Neumann, E. Miller, Y. Chen, R. G. Posner, Y. T. Lin and W. S. Hlavacek. Bayesian Inference with PyBioNetFit of State-Level R_0 Values for COVID-19 across the US. Presented at *q-bio Conference*, Fort Collins, Colorado, United States, 2022-06-15 - 2022-06-17. (LA-UR-22-25214)

**Peer-reviewed*

Solubility Enhanced High Surface Area Palladium/Carbon Materials for Helium3/ Tritium Separation

Rajinder Singh
20220290ER



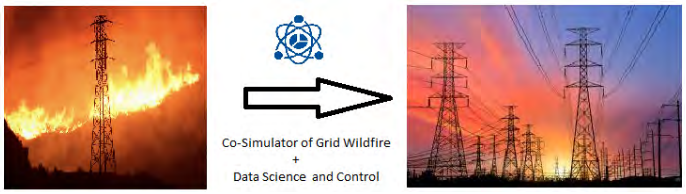
Tritium/Helium-3 separation from dilute gaseous streams is very challenging and currently use expensive palladium diffusers which are in short supply. Porous palladium-carbon hollow fibers present a structured radiation tolerant platform for efficient tritium/helium-3 separation leveraging the high affinity of palladium for hydrogen isotopes, high surface area packaging and efficient fluid dynamics.

Project Description

Helium-3 (3He) is critical for medical imaging (lung magnetic resonance imaging), nuclear security (radiation detectors), and scientific instruments (ultra-low temperature magnets). Since radioactive decay of tritium (T2) is the sole source of 3He on earth, the production of high purity 3He requires its extensive separation from T2 gas mixtures. Current state of the art palladium (Pd) diffuser technology has shortcomings to process streams with low concentration of T2. In addition, Pd diffuser technology is not readily available since the original manufacturer discontinued production. This project aims to develop novel porous carbon structured materials for efficient T2 separation from 3He/T2 gas mixtures. The structured packaging, high surface area and hierarchical morphology of the porous carbon platform together with enhanced T2 solubility in Pd will enable T2 capture and production of high purity 3He.

Resilient Operation of Interdependent Engineered Networks and Natural Systems

Deepjyoti Deka
20220371ER



The project aims to use data-science with a novel co-simuator tool to present the risk associated with wildfires on the power grid.

Project Description

Interdependent networked systems represent systems of great strategic importance, including modern infrastructure networks (transportation systems, power grids), and natural systems (climate systems, biological systems). Inter-dependencies between natural/physical systems and co-located man-made engineered systems impact the delivery of critical services. This project aims to study the complex interactions between the physics of a natural system and an engineered system with the goal of improving their robust and resilient operation. As a Los Alamos National Laboratory mission-specific use-case, this project concerns the mutual dependence between power grids and the spread of wildfires, and the effect of wildfire risk on human life and property. In this work, we propose to take a principled stochastic approach for the joint dynamics, and utilize this approach to determine optimal strategies to minimize the adverse impacts of system failures. It is essential to systematically understand the interaction between wildfires and electrical infrastructure to (a) conversely identify and minimize the wildfire risk posed by faulty electrical equipment, and (b) minimize the damage from spreading wildfires on critical infrastructure.

Publications

Journal Articles

Deka, D., r. wang, M. R. A. Paternina and W. Li. Physics-Constrained Adversarial Training for Neural Networks in Stochastic Power Grids. Submitted to *IEEE Transactions on Artificial Intelligence*. (LA-UR-23-20922)

Zhou, Y., K. Sundar, D. Deka and H. Zhu. Optimal Power System Topology Control Under Uncertain Wildfire Risk. Submitted to *IEEE Transactions on Smart Grid*. (LA-UR-23-22583)

Conference Papers

Li, W., K. Dvijotham and D. Deka. Physics-Constrained Interval Bound Propagation for Robustness Verifiable Neural Networks in Power Grids. Presented at *Workshop (W4): AI for Energy Innovation held in conjunction with 37th AAAI Conference on Artificial Intelligence (AAAI-23)*. (Washington, District Of Columbia, United States, 2023-02-13 - 2022-12-13). (LA-UR-23-20187)

Li, W. and D. Deka. PPGN: Physics-Preserved Graph Networks for Real-Time Fault Location in Distribution Systems with Limited Observation and Labels. Presented at *The Hawaii International Conference on System Sciences (HICSS)*. (Maui, Hawaii, United States, 2023-01-03 - 2023-01-06). (LA-UR-22-30465)

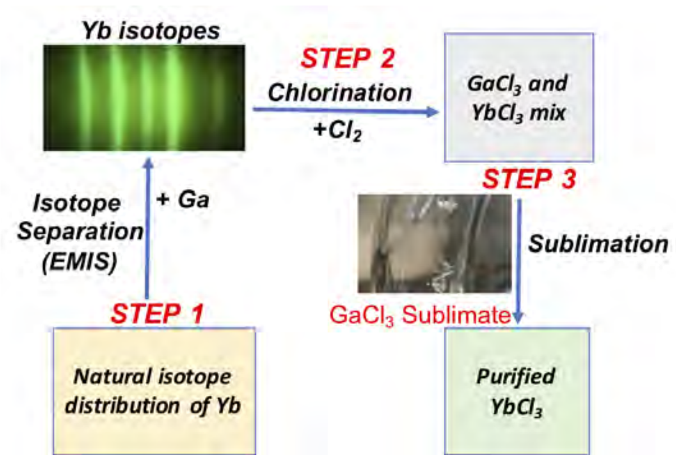
Presentation Slides

Li, W. and D. Deka. Physics-Informed Machine Learning for Enhancing Robustness and Verification. Presented at *NASPI Work Group Meeting & Vendor Show*, Tempe, Arizona, United States, 2023-04-04 - 2023-04-05. (LA-UR-23-23066)

**Peer-reviewed*

Sublimation for Rapid Isolation of Rare f-Element Isotopes

Aaron Tondreau
20220389ER



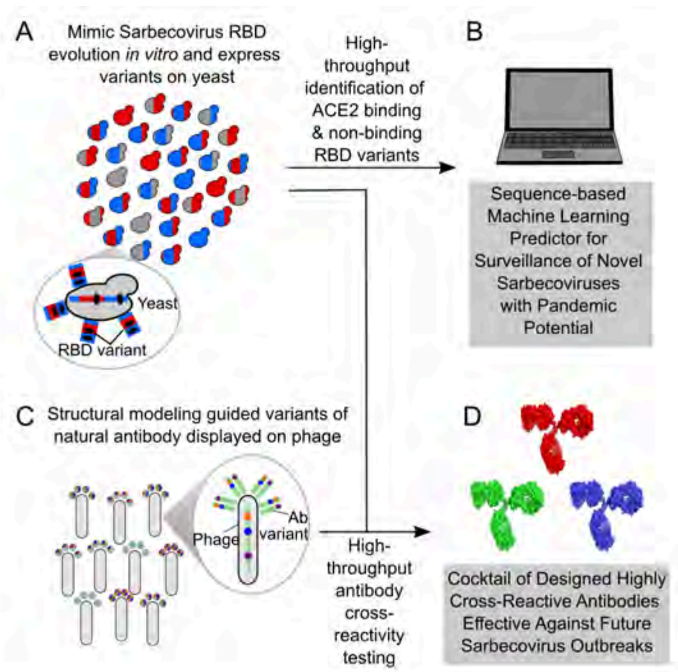
This proposal encompasses a three-step process. First is isotope separation of natural abundance ytterbium metal using an Electromagnetic Isotope Separator (EMIS). The separated isotopes are collected in a soft metal – gallium – to minimize material loss. Secondly, the formed gallium/ytterbium intermetallic undergoes complete chlorination into Ga/Yb trichloride materials. Finally, using the extremely different physical properties of the chloride materials, the gallium trichloride is removed by sublimation, leaving the non-volatile, purified YbCl3 behind.

Project Description

This project is designed to provide a new route to both isotopically and chemically purified lanthanide materials to lower United States dependence on foreign sources of these materials. Due to the implementation of a new technology of isotope separation technology, an opportunity to develop new separation technologies has presented itself, one where non-aqueous technologies can be employed. Aqueous work-ups generate liquid and column-material waste, and even easy separations using aqueous methods can take on the order of days to perform. This proposal aims to make large strides in circumventing aqueous processing. A new chemical process will be developed for isolation of isotopically pure lanthanides using stable isotopes of ytterbium (Yb). Ytterbium has immediate practical applications since the chemical methodologies will be developed for the recovery of high-value, isotopically pure isotopes 171Yb and more importantly 176Yb, used in the production of the medical isotope 177 Lutetium (177Lu).

In Vitro Evolution and Computational Approaches to Predict, Prevent, and Control Future Pandemics

Kshitij Wagh
20220399ER



(A) To mimic natural Sarbecovirus evolution, the project team will use in vitro evolution to generate ~10^8 RBD variants, which will be expressed on yeast for high-throughput profiling of binding to ACE2. (B) Using ACE2-binding and ACE2-non-binding RBD variant sequences, develop a machine learning predictor for ACE2 binding that will help identify animal Sarbecoviruses of pandemic concern. (C) To design cross-reactive antibodies, the team will express ~10^6 structural modeling guided antibody variants on phage, and identify cross-reactive antibodies by high-throughput binding to the RBD-yeast library. (D) Design a cocktail of 2-3 highly cross-reactive antibodies to mitigate future Sarbecovirus outbreaks.

Project Description

The coronavirus (COVID-19) pandemic has underscored the devastation caused by novel animal virus “spillovers” into humans. Thus, pandemic preparedness is paramount, but the unpredictability of which animal virus can next infect humans severely restricts such efforts. To overcome this limitation, we will develop experimental and computational strategies that can help predict, prevent, and control future pandemics. For proof of concept, we will focus on the Coronavirus family that gave rise to the Severe Acute Respiratory Syndrome (SARS) and COVID-19 pandemics. We will first develop a novel strategy to predict whether a new animal Coronavirus can bind to the entry protein on human cells, the first step in infection. This research can facilitate high-throughput surveillance of animal Coronaviruses of pandemic concern, and could help prevent new Coronavirus outbreaks. Second, we will design antibodies that can be broadly effective against animal Coronaviruses with pandemic potential. Such antibodies could be used as the first-line-of-defense drugs to dampen the initial spread of future Coronavirus outbreaks, and prevent the escalation to global pandemics. Because pandemics have significant global health, socioeconomic and national security impacts, our pandemic preparedness research will fulfill the missions of Los Alamos National Laboratory, Department of Energy Office of Science Biological and Environmental Research, and the National Security Life Sciences initiative.

Publications

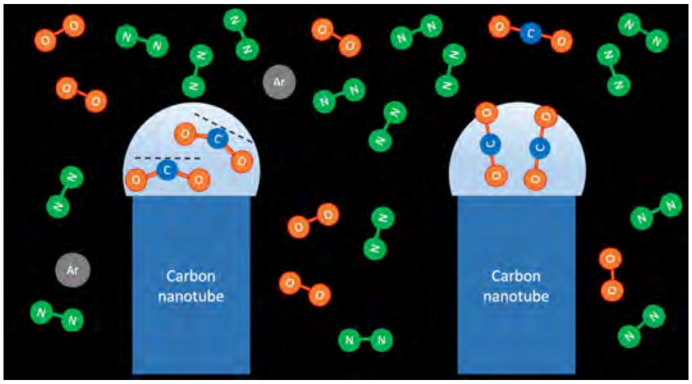
Journal Articles

Dagotto, G., J. D. Ventura, D. R. Martinez, T. Anioke, B. S. Chung, M. Siamatu, J. Barrett, J. Miller, A. Schafer, J. Yu, L. H. Tostanoski, K. Wagh, R. S. Baric, B. Korber and D. H. Barouch. Immunogenicity and protective efficacy of a rhesus adenoviral vaccine targeting conserved COVID-19 replication transcription complex. 2022. *npj Vaccines*. **7** (1): 125. (LA-UR-22-31546 DOI: 10.1038/s41541-022-00553-2)

**Peer-reviewed*

Direct Air Capture of CO2 Using Reversible Electrostatic Interactions

Alp Findikoglu
20220738ER



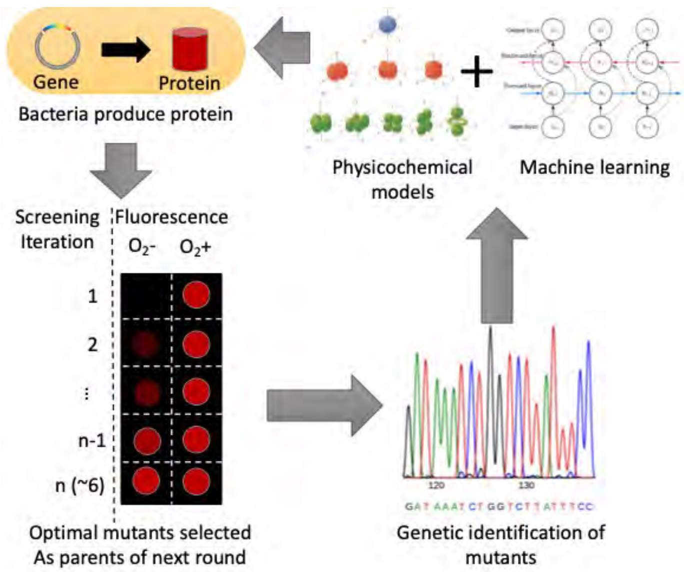
Schematic depiction of electrostatic direct air capture (DAC) of CO2 using large electric field gradients at the tip of carbon nanotubes, where both induced dipole and permanent quadrupole interactions with the biased electrode are considered

Project Description

The proposed project aims to demonstrate a disruptive process for energy-efficient, reversible direct air capture (DAC) of carbon dioxide (CO2). DAC of CO2 is a growing field that is urgently searching for cost-effective and globally scalable technologies to reduce the potentially disastrous effects of global warming. The proposed approach has the potential to provide a unique solution to this long-standing problem by demonstrating the capture and release at room temperature of CO2 reversibly, akin to charging and discharging of a capacitor, for a paradigm shift in energy efficient removal of CO2 from the atmosphere.

Lighting up Oxygen-Free Biology with Next Generation Fluorescent Proteins

Shounak Banerjee
20220743ER



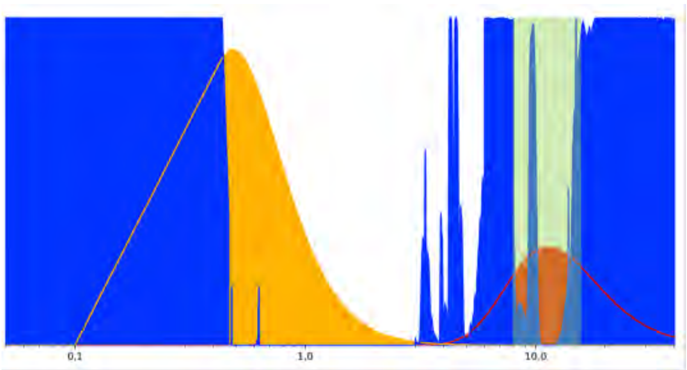
High throughput screening and selection of next generation, oxygen independent fluorescent proteins is performed by generating several thousand mutants of an existing fluorescent protein, screening these in an oxygen deficient environment, selecting the best performing (eg. brightest) mutants, interbreeding their sequences and producing successive and even better performing "offspring" proteins. Computational models are used to analyze the effects of different mutations and predict additional mutations to introduce into the interbreeding step.

Project Description

Several aspects of oxygen-deprived and oxygen-free biology remain poorly understood owing to the lack of biological tools to visualize phenomena. This precludes the development of several high-throughput artificial evolution protocols for biological engineering projects related to food, energy and environmental security. These are some of the core missions of the Department of Energy (DOE) Offices of Science, Applied Energy, Advanced Manufacturing, Bioenergy Technologies and hydrogen fuel technologies. We envision our technology to be enabling and transformational to several ongoing funded projects and future opportunities for the above DOE entities. The most immediate effects will be seen on projects relating to deconstruction and upcycling of petroleum based plastics, waste stream valorization, renewable fuel production and carbon negative manufacturing processes enabled by micro-organisms that are unable to survive even small quantities of oxygen.

Biologically Cooling the Planet: A BRISK Approach that Directly Connects the Ground to Deep Space

Murray Wolinsky
20220769ER



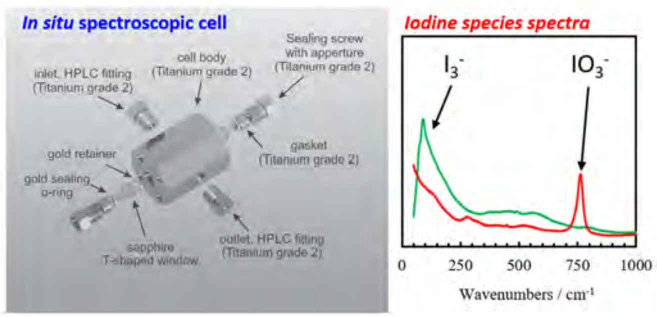
We want to determine how well biological organisms can exploit a window in the earth's atmospheric absorption spectrum (shown in light green to provide useful cooling.

Project Description

Combatting climate change is vital to both national and global security and therefore to Laboratory mission. As Earth warms, oceans rise, food becomes scarcer and pathogens more prevalent. People are displaced. Conflicts intensify. Our military factors all these concerns into its plans. Our proposed work identifies a novel approach to these problems. Specifically, we want to understand whether plants can significantly offset warming using only the ambient thermal environment, The mechanism we will study is called radiative sky cooling. It exploits a "hole" in the atmospheric absorption spectrum which permits heat to reach cold deep space without warming the air. Our proposal asks an important (and not yet studied) fundamental scientific research question and opens a door to possible long-term continued funding for significant science and engineering application development.

Hydrothermal Iodine Chemistry for Nuclear Event Detection

Chelsea Neil
20220777ER



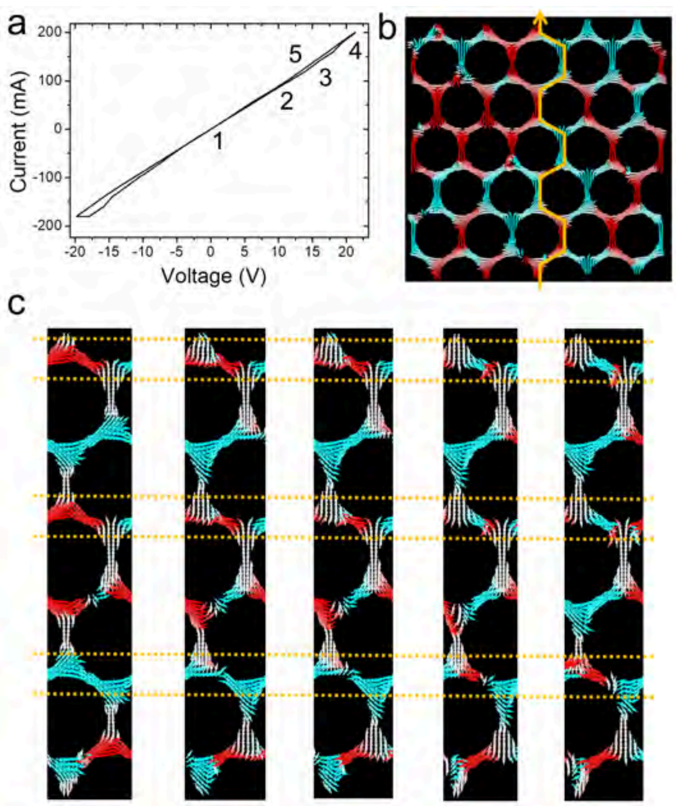
In situ spectroscopic techniques are powerful tools for distinguishing between iodine oxidation states, for example discriminating the oxidized IO3- from the reduced I3-. In the proposed work, the team will take advantage of this ability by integrating established in situ specstrocopic cells with redox control capability to make measurements of iodine speciation under controlled redox conditions.

Project Description

Radiochemical signatures such as radioxenon isotopic ratios are considered a smoking gun for underground nuclear detonation detection. However, accurate interpretation of detected radioxenon signatures necessitates a complete understanding of the various transport processes which bring these signatures from their source (i.e., an underground cavity) to the point of detection. Within this system, significant uncertainty stems from the near-cavity hydrothermal chemistry of iodine, an abundant fission product and the direct precursor to xenon in the nuclear decay chain. Iodine can exist as multiple chemical forms, and these forms will directly impact its transport and reactivity in the subsurface. The project will develop a new cell which can be used to observe iodine chemical form under controlled environmental conditions. A better understanding of post-underground nuclear explosion iodine transport will improve our ability to attribute the source of detected radioxenon isotopes, a critical component of proliferation monitoring.

Passive MemComputing in Lithographic Arrays of Interacting Magnetic Nanoislands

Francesco Caravelli
20200105ER



The figure represents the magnetic structure of a Kagome spin ice, and the yellow part (top right) represents the flow of the currents. At different time steps (see bottom figure) the magnetic states of the material change depending on the current, and so does the resistive state. This can be seen from the widening of the I-V plot (top left) as a function of current and a cyclical voltage. This implies memory, which is due to the magnetic coupling to local currents.

Project Description

The brain is estimated to perform up to 100 trillion TEPS (Traversed Edges Per Second) at a cost of approximately 20-25 Watts in energy. The Department of Energy (DOE) BlueGene supercomputer performs roughly 10 times fewer operations, but to do so it requires more than 10,000 times the energy. We propose to overcome that limitation via memcomputing. The concept of memcomputing is a general approach to beyond-Turing-machine computation that has been identified by DOE as an essential national security challenge.

Technical Outcomes

One of the advantages of using magnetic devices is that they can operate near the Landauer limit, and thus use the minimum amount of energy consumption per energy bit. The project used a variety of computational methods to embed computational problems into magnetic and spin ice materials, and this project lead to various proof of principles, ranging from embedding neural networks to reservoir computers.

Publications

Journal Articles

Caravelli, F. Botanic approximations to two-body partition functions for sparse graphs. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-20-24400)

*Caravelli, F. Some exactly solvable and tunable frustrated spin models. 2022. *Physica A: Statistical Mechanics and its Applications*. **594**: 127007. (LA-UR-21-30815 DOI: 10.1016/j.physa.2022.127007)

Caravelli, F., F. Traversa, M. Bonnin and F. Bonani. Projective Embedding of Dynamical Systems: uniform mean field equations. Submitted to *International Journal of Nonlinear Sciences and Numerical Simulations*. (LA-UR-21-29420)

Caravelli, F., G. Milano, C. Ricciardi and Z. Kuncic. Conductance transitions in Ag-nanowire connectome. Submitted to *PNAS*. (LA-UR-22-28057)

Caravelli, F., J. Gartside, W. Bramford, H. Kurebayashi, K. Stenning, H. Holder, T. Dion and D. Arroo. Reconfigurable Training and Reservoir Computing in an Artificial Spin-Vortex Ice via Spin-Wave Fingerprinting. Submitted to *Nature Nanotechnology*. (LA-UR-22-30378)

Caravelli, F., M. D. Saccone, J. Gartside, W. Bramford and K. Stelling. From vertices to vortices in magnetic nanoislands. 2023. *Physics of Fluids*. **35** (1): 017101. (LA-UR-22-28056 DOI: 10.1063/5.0131158)

*Caravelli, F., M. Saccone and C. Nisoli. On the degeneracy of spin ice graphs, and its estimate via the Bethe permanent. 2021. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*. **477** (2252): 20210108. (LA-UR-21-20434 DOI: 10.1098/rspa.2021.0108)

Caravelli, F. and C. Nisoli. Mean Field Spin Ice on arbitrary graphs:\\\\ analysis of static and dynamic equations. Submitted to *Physical Review E*. (LA-UR-20-24401)

*Caravelli, F. and C. Nisoli. Logical gates embedding in artificial spin ice. 2020. *New Journal of Physics*. **22** (10): 103052. (LA-UR-20-28537 DOI: 10.1088/1367-2630/abbf21)

Caravelli, F. and F. C. Sheldon. Phases of memristive circuits via an interacting disorder approach. Submitted to *Physical Review E*. (LA-UR-20-24399)

*Duzgun, A., A. Saxena and J. V. Selinger. Alignment-induced reconfigurable walls for patterning and assembly of liquid crystal skyrmions. 2021. *Physical Review Research*. **3** (1): L012005. (LA-UR-20-20733 DOI: 10.1103/PhysRevResearch.3.L012005)

J. Fonseca, W. B., F. Garcia, F. Caravelli and C. de Araujo. Memristive effects in nanopatterned permalloy Kagome array. Submitted to *Physical Review Applied*. (LA-UR-21-30859)

*Hofhuis, K., C. F. Petersen, M. Saccone, S. Dhuey, A. Kleibert, S. van Dijken and A. Farhan. Geometrical frustration and competing orders in the dipolar trimerized triangular lattice. 2021. *Physical Review B*. **104** (1): 014409. (LA-UR-21-23310 DOI: 10.1103/PhysRevB.104.014409)

*King, A., C. Nisoli and A. Lopez-Bezanilla. Qubit spin ice. 2021. *Science*. **373** (6554): 576-580. (LA-UR-20-30163 DOI: 10.1126/science.abe2824)

Lopez-Bezanilla, A., J. Raymond, C. Nisoli and A. King. Kagome qubit ice. Submitted to *Nature Communications*. (LA-UR-22-27029)

*May, A., M. Saccone, A. van den Berg, J. Askey, M. Hunt and S. Ladak. Magnetic charge propagation upon a 3D artificial spin-ice. 2021. *Nature Communications*. **12** (1): 3217. (LA-UR-21-22700 DOI: 10.1038/s41467-021-23480-7)

Merrigan, C., D. Shohat, C. Sirote, Y. Lahini, C. Nisoli and Y. Shokef. Emergent Disorder and Mechanical Memory in Periodic Metamaterials. Submitted to *Physical Review Letters*. (LA-UR-22-27017)

Merrigan, C., Y. Shokef and C. Nisoli. Topologically protected steady cycles in an icelike mechanical metamaterial. Submitted to *Physical Review Research*. (LA-UR-20-28310)

Pisanty, B., E. Oguz, C. Nisoli and Y. Shokef. Putting a spin on metamaterials: Mechanical incompatibility as magnetic frustration. Submitted to *SciPost Physics*. (LA-UR-20-28535)

Saccone, M. D., A. Van den Berg, E. Harding, S. Singh, S. R. Giblin, F. Flicker and S. Ladak. Exploring the phases of 3D artificial spin ice: From Coulomb phase to magnetic monopole crystal. Submitted to *Nature Physics*. (LA-UR-22-32126)

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Saccone, M. D. and F. Caravelli. Complex field reversal dynamics in nanomagnetic systems. Submitted to *Proceedings of the Royal Society A. Mathematical, Physical and Engineering Sciences*. (LA-UR-23-21161)

*Saccone, M., F. Caravelli, K. Hofhuis, S. Parchenko, Y. A. Birkhoelzer, S. Dhuey, A. Kleibert, S. van Dijken, C. Nisoli and A. Farhan. Direct observation of a dynamical glass transition in a nanomagnetic artificial Hopfield network. 2022. *Nature Physics*. **18** (5): 517-521. (LA-UR-21-27055 DOI: 10.1038/s41567-022-01538-7)

*Saccone, M., F. Caravelli, K. Hofhuis, S. Parchenko, Y. A. Birkhoelzer, S. Dhuey, A. Kleibert, S. van Dijken, C. Nisoli and A. Farhan. Direct observation of a dynamical glass transition in a nanomagnetic artificial Hopfield network. 2022. *Nature Physics*. **18** (5): 517-521. (LA-UR-21-28829 DOI: 10.1038/s41567-022-01538-7)

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Sheldon, F. C., F. Caravelli and A. Kolchinsky. Feasibility, Optimality and Implementability of memory circuits for Reservoir Computing. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-20314)

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Teixeira, H. A., M. F. Bernardo, F. Caravelli, M. D. Saccone, C. Nisoli and C. I. L. Araujio. Macroscopic Magnetic Monopoles in a 3D-Printed Mechano-Magnet. Submitted to *PNAS*. (LA-UR-22-20185)

*Yue, W., Z. Yuan, Y. Lyu, S. Dong, J. Zhou, Z. Xiao, L. He, X. Tu, Y. Dong, H. Wang, W. Xu, L. Kang, P. Wu, C. Nisoli, W. Kwok and Y. -. Wang. Crystallizing Kagome Artificial Spin Ice. 2022. *Physical Review Letters*. **129** (5): 057202. (LA-UR-22-20182 DOI: 10.1103/PhysRevLett.129.057202)

*D. A. *. L. Y. *. S. S. *. B. N. S. *. S. J. *. S. H. *. R. J. *. B. J. T. *. W. J. D. *. B. D. *. C. R. V. *. O. L. *. L. C. *. N. C. *. S. P. Zhang, X. *., A. Duzgun and C. Nisoli. String Phase in an Artificial Spin Ice. 2021. *Nature Communications*. **12** (1): 6514. (LA-UR-20-24782 DOI: 10.1038/s41467-021-26734-6)

Zhang, X., G. Fitez, S. Subzwari, N. Bingham, I. Chioar, H. Saglam, J. Ramberger, C. Leighton, C. Nisoli and P. Schiffer. Topological Kinetic Crossover in a Nanomagnet Array. Submitted to *Science*. (LA-UR-22-27019)

Books/Chapters

Nisoli, C. Elliott Lieb, Vertex Models, and Artificial Spin Ice. (LA-UR-22-21460)

Presentation Slides

Caravelli, F. Computing with memristive devices and networks. . (LA-UR-20-29551)

Caravelli, F. Computing within spin ice. . (LA-UR-20-29596)

Caravelli, F. Locality of centrality measures of networks. Presented at *Complex Networks 2021*, Barcelona, Spain, 2021-11-30 - 2021-12-02. (LA-UR-21-31159)

Caravelli, F. Computing with Spin Ice. . (LA-UR-22-20331)

Casleton, E. M. Organizational Description. Presented at *Women in Statistics and Data Science Conference*, St. Louis, Missouri, United States, 2022-10-06 - 2022-10-06. (LA-UR-22-29093)

Saccone, M. D. and F. Caravelli. How nanomagnets process information. Presented at *MMM 2022*, Minneapolis, Minnesota, United States, 2022-10-31 - 2022-10-31. (LA-UR-22-31280)

Posters

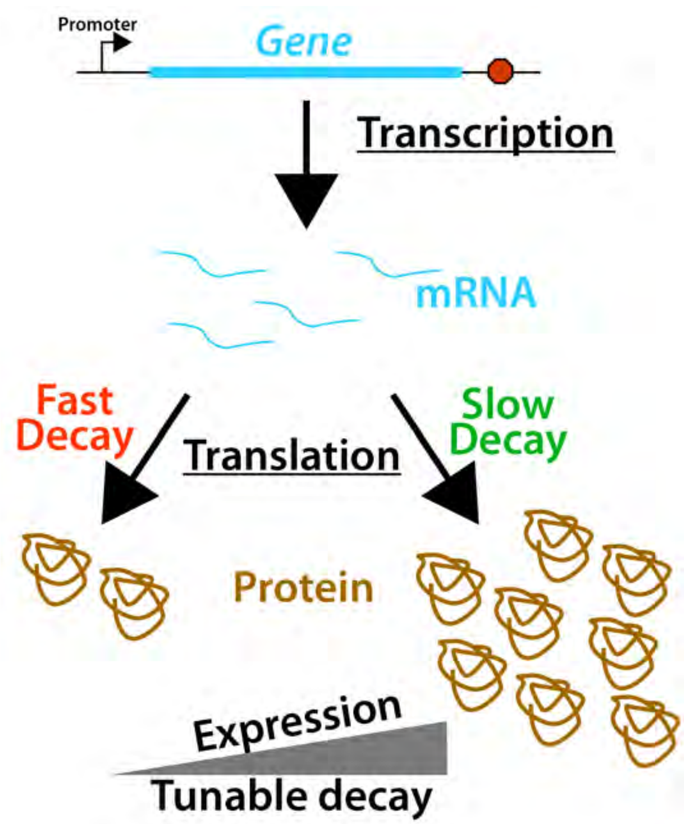
Caravelli, F. The odd 8-vertex model via Fisher-Dub\\'{e}dat decorations. Presented at *Waiting for frustrated magnetism*, Some city in germany, Germany, 2021-01-20 - 2021-01-25. (LA-UR-21-20473)

Caravelli, F. PHASE TRANSITIONS IN DISORDERD CIRCUITS WITH MEMORY. Presented at *MECO 47*, Erice, Italy, 2022-06-06 - 2022-06-07. (LA-UR-22-24881)

**Peer-reviewed*

Reshaping Bacterial Metabolic Output by Deciphering the Determinants of Messenger RiboNucleic Acid (mRNA) Decay

Christina Steadman
20200111ER



mRNA decay is an important mechanism of genetic regulation. However, the rules governing enhanced stability and differential decay are not fully understood. In this research the project team is using next-generation sequencing, genomic engineering, and novel computational analysis method to uncover the motifs in RNA transcripts that can afford differential stabilities spanning orders of magnitude.

Project Description

This project addresses global warming and energy security challenges. Metabolic engineering of microbes using synthetic biology techniques holds great promise for the carbon-neutral production of biofuels and many industrially relevant high-value commodity chemicals and precursors. This project aims to understand, in greater detail than previously possible, a fundamental aspect of bacterial physiology. The information will have immediate utility in re-wiring bacterial metabolism to maximize production of desirable compounds. The goal is to understand RiboNucleic Acid (RNA) metabolism, a primary determinant of the proteome, and therefore the metabolic profile of a given organism. Bacteria utilize the stability of Messenger RNA (mRNA) to titrate the production of specific proteins. This process remains cryptic and our intent is to uncover the mechanisms whereby RNAs are either stabilized or destabilized. We will create models with sufficient detail to allow the encoding of new pathways that redirect carbon and energy toward a novel end product while preserving growth and viability.

Technical Outcomes

Ribonucleic acid (RNA) metabolism is an important facet of biology that requires deeper understanding for synthetic bioengineering outcomes ranging from bioenergy to biosecurity applications. In this project, the team developed the capability for ascertaining the features that contribute to the stability of RNA. This capability includes novel experimental and computational toolkits for using Nanopore sequencing platform, which is advantageous over traditional sequencing. The team analyzed RNA degradation and found determinants of RNA stability.

Publications

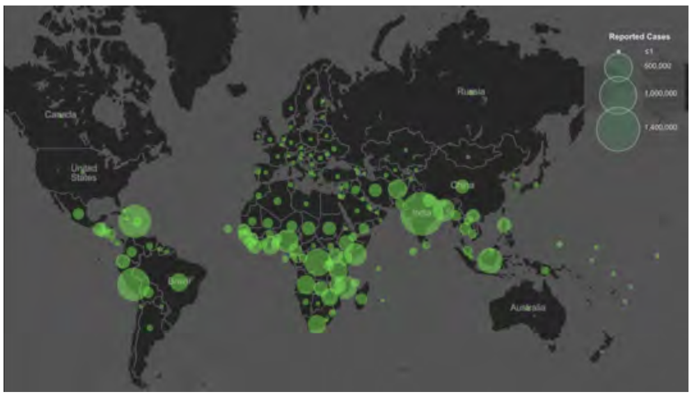
Journal Articles

Nemashkalo, A., M. E. Phipps, S. P. Hennelly and P. M. Goodwin. Real-time single molecule observation of biomolecular interactions inside nanophotonic zero mode waveguides. Submitted to *IOP Nanotechnology Special Issue*. (LA-UR-21-28847)

**Peer-reviewed*

The Genetic Patterns of Migration in Global Pandemics

Andrey Lokhov
20200121ER



This figure illustrates the spread of cholera in the world, which continues to be a global threat, causing 4 million cases and 150,000 deaths per year. This projects attempts to quantitatively understand the global spread of cholera and its relation to migration by developing learning algorithms that use both traditional case counts, as well as genomic data. By exploiting the accumulation of mutations in genetic sequences over time, the team will attempt to test a hypothesis that cholera transmission is not locally sustainable in parts of the world and that outbreaks are caused by periodic re-seeding from long-range transmission events.

Project Description

We will focus on the bacterium Vibrio cholerae which causes 4 million cases of cholera and 150,000 deaths per year. For V. cholerae, there are both endemic (e.g. South Asia) and epidemic regions (e.g., sub-Saharan Africa and Middle East) that are linked by economic and cultural migration. We believe that cholera transmission is not locally sustainable in parts of the world and that outbreaks are caused by periodic re-seeding from long-range transmission events. Demonstrating this will open up new options for global control of cholera such as targeted vaccination at global source hot spots. Existing work on global patterns of mutation and migration generally either use genetic sequence data as a kind of simple partition of patients into subtypes, or indirectly use the inferred phylogeny (a representation of evolutionary history as a binary tree) only for making claims based on an implicit clustering pattern. Network structure and transmission parameters will be investigated using genetic sequence data and country-level time series of infected cases and will expand the Laboratory's capacity for using growing global repositories of pathogen sequence data for defining and mitigating national security bio-threats.

Technical Outcomes

The successful results of this project presented convincing evidence that phylodynamic methods can be used to study cholera outbreaks at a regional level and that they produce parameter estimates that are consistent with established methods. The team's approach provided a common methodology for an early analysis of the model viability in the context of joint inference from different data sources.

Publications

Journal Articles

*Cu\xc3\xa9llar, L., I. Torres, E. Romero-Severson, R. Mahesh, N. Ortega, S. Pungitore, R. Ke and N. Hengartner. Assessing the impact of human mobility to predict regional excess death in Ecuador. 2022. *Scientific Reports*. **12** (1): 370. (LA-UR-21-21098 DOI: 10.1038/s41598-021-03926-0)

Gajewski, \. G., J. Cho\xc5\x82oniewski and M. J. Wilinski. Detecting Hidden Layers from Spreading Dynamics on Complex Networks. Submitted to *Physical Review E*. (LA-UR-21-21525)

Li, B., D. Saad and A. Lokhov. Reducing Urban Traffic Congestion Due To Localized Routing Decisions. Submitted to *Physical Review Letters*. (LA-UR-20-22351)

*Romero-Severson, E. O., N. Hengartner, G. Meadors and R. Ke. Change in global transmission rates of COVID-19 through May 6 2020. 2020. *PLOS ONE*. **15** (8). (LA-UR-20-23673 DOI: 10.1371/journal.pone.0236776)

*Snyder, J., A. Zlotnik and A. Y. Lokhov. Data-driven selection of coarse-grained models of coupled oscillators. 2020. *Physical Review Research*. **2** (4): 043402. (LA-UR-20-27371 DOI: 10.1103/PhysRevResearch.2.043402)

Sun, H., D. Saad and A. Lokhov. Competition, Collaboration, and Optimization in Multiple Interacting Spreading Processes. Submitted to *Physical Review X*. (LA-UR-20-28394)

Wilinski, M. J., L. A. Castro, J. S. Keithley, C. A. Manore, J. Campos, E. Romero-Severson, D. Domman and A. Lokhov. Congruity of genomic and epidemiological data in modeling of local cholera outbreaks. Submitted to *Nature Communications*. (LA-UR-22-30152)

Conference Papers

Dutt, A., A. Lokhov, M. D. Vuffray and S. Misra. Exponential Reduction in Sample Complexity with Learning of Ising Model Dynamics. Presented at *NeurIPS*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-24926)

Dutt, A., A. Lokhov, M. D. Vuffray and S. Misra. Exponential Reduction in Sample Complexity with Learning of Ising Model Dynamics. Presented at *International Conference on Machine Learning (ICML)*. (Online, New Mexico, United States, 2021-07-18 - 2021-07-24). (LA-UR-21-21523)

Lokhov, A., S. Misra, C. X. Ren and M. D. Vuffray. Learning Continuous Exponential Families Beyond Gaussian. Presented at *International Conference on Machine Learning (ICML)*. (Online, New Mexico, United States, 2021-07-18 - 2021-07-24). (LA-UR-21-21520)

Lokhov, A. and D. Saad. Scalable Influence Estimation Without Sampling. Presented at *ECML PKDD 2020*. (Ghent, Belgium, 2020-09-14 - 2020-09-14). (LA-UR-20-22301)

Lokhov, A. and M. J. Wilinski. Scalable Learning of Independent Cascade Dynamics from Partial Observations. Presented at *International Conference on Machine Learning (ICML)*. (Online, New Mexico, United States, 2021-07-18 - 2021-07-24). (LA-UR-21-21521)

Misra, S., M. D. Vuffray and A. Lokhov. Information Theoretic Optimal Learning of Gaussian Graphical Models. Presented at *Conference on Learning Theory*. (Online, New Mexico, United States, 2020-07-09 - 2020-07-09). (LA-UR-20-24929)

Ren, C. X., S. Misra, M. D. Vuffray and A. Lokhov. Learning Continuous Exponential Families Beyond Gaussian. Presented at *NeurIPS 2022*. (New Orleans, Louisiana, United States, 2022-11-28 - 2022-11-28). (LA-UR-22-25979)

Wilinski, M. and A. Lokhov. Scalable Learning of Independent Cascade Dynamics from Partial Observations. Presented at *NeurIPS*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-24928)

Presentation Slides

Lokhov, A. The Genetic Patterns of Migration in Global Pandemics. . (LA-UR-20-29787)

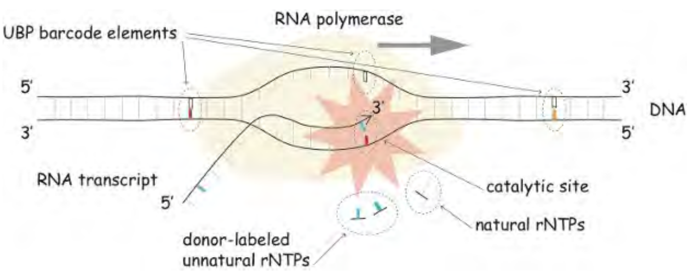
Lokhov, A. Prediction-Centric Learning of Independent Cascade Dynamics from Partial Observations. Presented at *Conference on Complex Systems*, Lyon, France, 2021-10-25 - 2021-10-29. (LA-UR-21-30706)

Wilinski, M. J. Prediction-Centric Learning of Spreading Dynamics from Partial and Noisy Observations. Presented at *Physics Informed Machine Learning 2022*, Santa Fe, New Mexico, United States, 2022-05-11 - 2022-05-13. (LA-UR-22-24811)

**Peer-reviewed*

Observing Life: Real-time Imaging of Transcription Using Unnatural Base-Pairs in Living Cells

Jurgen Schmidt
20200161ER



Fluorescence resonance energy transfer (FRET) detection of RNA transcription using donor- and acceptor-labeled unnatural base pairs (UPBs). During RNA polymerase catalyzed transcription of DNA to RNA, incorporation of the donor-labeled rNTP base (blue) into the growing RNA strand brings the donor fluorophore into close proximity of the cognate acceptor fluorophore-labeled base (red) incorporated in the template DNA strand resulting in FRET generated acceptor fluorescence. The goal of this project is to develop the needed reagents (fluorophore-labeled unnatural DNA and RNA bases, and engineered DNA and RNA polymerase) to enable sensitive, real-time detection of single transcription events in vivo.

Project Description

Life is the sum total of a myriad of large and small regulatory transitions. To date, the dynamics of these processes have been inaccessible. The development of our synthetic biology technology will allow real-time single-cell imaging of gene transcription in living cells. Unnatural nucleotide bases in semi-synthetic organisms create barcodes at specific sites in the genome. Ultimately this technology will provide unprecedented access to the dynamics of the transcription of multiple genes in single living cells. As regulated gene expression is the basis of all cellular processes, we will be able to observe and quantify the fundamental dynamics of life. The potential applications of, and new insights provided by, this new imaging modality are immense: mapping of any signaling pathway activity (e.g. metabolic and lineage specification pathways), oncogene activity in cancer cells, biological systems interactions and basic gene regulation principles, cellular response to stimuli. The ability to visualize transcription at the single-cell level in real-time will provide unprecedented insights of cellular activity with wide-ranging, enabling impact on national security and threat science to public health and energy security.

Technical Outcomes

The project team developed novel synthetic robust routes to unnatural base pair nucleosides, a new auto-fluorescent detection method and screened polymerases for the replication of these unnatural nucleoside containing oligomers. The project seeded critical expertise that is currently deployed on the evaluation of novel nucleoside biomolecular tools and the implications of unnatural codes for information storage.

Publications

Journal Articles

*Pace, N. A., S. P. Hennelly and P. M. Goodwin. Immobilization of Cyanines in DNA Produces Systematic Increases in Fluorescence Intensity. 2021. *The Journal of Physical Chemistry Letters*. **12** (37): 8963-8971. (LA-UR-21-25758 DOI: 10.1021/acs.jpclett.1c02022)

Presentation Slides

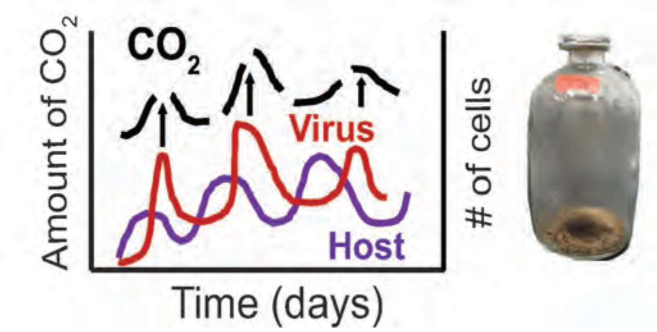
Corbin, J. R., R. Wu and J. G. Schmidt. Synthetic Chemistry to Support RIVOT. Presented at *Workshop on Visualizing Living Systems*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21866)

Pace, N. A., P. M. Goodwin, S. P. Hennelly and R. Wu. FRET Gate for Real-Time In-Vivo Transcription. Presented at *Visualizing Living Systems Workshop*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22692)

**Peer-reviewed*

Small Things Considered: Are Viruses as Important to Carbon Cycling in Soils as in Oceans?

Migun Shakya
20200252ER



A current focus of Carbon (C) cycle model improvement is the discovery and inclusion of microbial processes that impact C cycling. A major process that has been previously ignored in terrestrial systems is virus-induced microbial mortality. Our project characterizes the impact of viruses in driving C cycling dynamics in soil ecosystems. The approach combines experimental ecology, traditional microbiology, advanced 'omic' technologies, and computational techniques to link virus-host dynamics with soil ecosystem function.

Project Description

Predicting the effects of climate change is a National and Global Security mission. Understanding carbon (C) cycling in terrestrial ecosystems, which are responsible for ~50% of carbon dioxide (CO2) emissions, is central to this mission. Accurate models of C flow in Earth systems are pivotal. However, large unexplained variance in C cycle models and poor spatial correlation of predicted and observed terrestrial C stocks create substantial uncertainty in predictions of C cycling. A current focus of model improvement is discovery and inclusion of microbial processes that impact C cycling, where microbes contribute to half (60 gigatonne) of C efflux in the terrestrial biosphere. A major process that has been previously ignored is virus-induced microbial mortality, which is somewhat analogous to insect-driven forest mortality. To inform modeling and ecosystem management, this project will begin to characterize the impact of viruses in driving C cycling dynamics of soil ecosystems.

Technical Outcomes

The project was successful in achieving goals through experiments in both environment and laboratory settings. The team developed novel methods to extract viruses from soil, track their dynamic in laboratory microcosm, sequence, and characterize their sequenced genomes, which enabled discovery of thousands of novel viruses and obtain direct evidence of effects of virus in environmental microbiomes as it relates to carbon cycle. New capabilities and findings puts us in position for large scale experiments.

Publications

Journal Articles

N. Albright, M. B., L. A. Gallegos-Graves, K. L. Feeser, K. N. Montoya, J. Emerson, M. Shakya and J. M. Dunbar. Experimental evidence for the impact of soil virus abundance on carbon cycling during surface plant litter decomposition. Submitted to *ISME Journal*. (LA-UR-21-28749)

Ball, B., P. Convey, K. L. Feeser, U. N. Nielsen and D. Van Horn. Habitat severity characteristics structure soil communities at regional and local spatial scales along the Antarctica Peninsula. Submitted to *Antarctic Science*. (LA-UR-23-23087)

Ball, B., P. Convey, K. L. Feeser, U. N. Nielsen and D. Van Horn. Environmental harshness mediates the relationship between aboveground and belowground communities in Antarctica. Submitted to *Soil Biology & Biochemistry*. (LA-UR-23-23088)

Jiang, X., D. Van Horn, J. G. Okie, H. Buelow, E. Schwartz, D. Colman, K. L. Feeser and C. Takacs-Vesbach. Limits to the three domains of life: lessons from community assembly along an Antarctic salinity gradient. Submitted to *Extremophiles*. (LA-UR-23-23086)

*Marti-Carreras, J., A. R. Gener, S. D. Miller, A. F. Brito, C. E. Camacho, R. Connor, W. Deboutte, C. Glickman, D. M. Kristensen, W. K. Meyer, S. Modha, A. L. Norris, S. Saha, A. K. Belford, E. Biederstedt, J. R. Brister, J. P. Buchmann, N. P. Cooley, R. A. Edwards, K. Javkar, M. Muchow, H. S. Muralidharan, C. Pepe-Ranney, N. Shah, M. Shakya, M. J. Tisza, B. J. Tully, B. Vanmechelen, V. C. Virta, J. L. Weissman, V. Zalunin, A. Efremov and B. Busby. NCBI's Virus Discovery Codeathon: Building "FIVE" —The Federated Index of Viral Experiments API Index. 2020. *Viruses*. **12** (12): 1424. (LA-UR-20-23300 DOI: 10.3390/v12121424)

Reports

Shakya, M. Los Alamos LDRD Report: Small Things Considered: Are Viruses as Important to Carbon Cycling in Soils as in Oceans?. Unpublished report. (LA-UR-22-30104)

Presentation Slides

Feeser, K. L., E. A. Middlebrook, B. J. Youtsey, L. A. Gallegos-Graves, M. B. N. Albright, J. M. Dunbar and M. Shakya. Soil viral community dynamics along a naturally occurring organic carbon gradient in a temperate desert. Presented at *Annual Sequencing, Finishing, and Analysis in the Future (SFAF) Conference*, Santa Fe, New Mexico, United States, 2022-06-21 - 2022-06-23. (LA-UR-22-25744)

Shakya, M., E. Tran, M. B. N. Albright and K. L. Feeser. Genomic and functional diversity of viruses in soils from New Mexico. Presented at *Phages for Health & Energy Symposium*, Virtual, New Mexico, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-29371)

Shakya, M., E. Tran and M. B. N. Albright. How does the environment affect prophages? Characterizing prophages from various environments to understand their distribution. Presented at *LANL student symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27521)

Shakya, M., K. L. Feeser, N. D. Ruth and B. J. Youtsey. Soil viral community dynamics along a naturally occurring organic carbon gradient in temperate desert. Presented at *Los Alamos Arizona day*, Los Alamos, New Mexico, United States, 2022-08-15 - 2022-08-15. (LA-UR-22-28564)

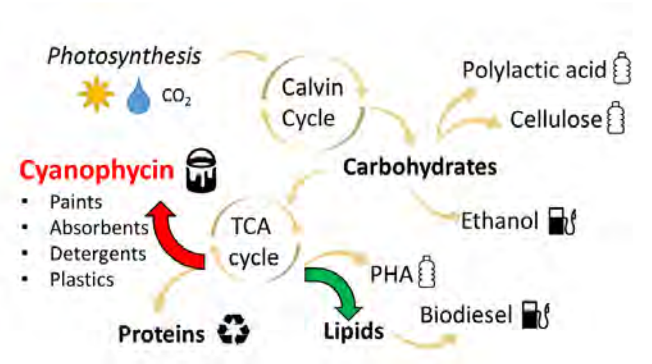
Posters

N. Albright, M. B., L. A. Gallegos-Graves, K. L. Feeser, J. Emerson, M. Shakya and J. M. Dunbar. Impact of Soil Viruses on Carbon Cycling. Presented at *VEGA symposium*, Los Alamos, New Mexico, United States, 2021-05-13 - 2021-05-13. (LA-UR-21-24389)

**Peer-reviewed*

Engineering Green Factories for the Production of Renewable Chemicals

Taraka Dale
20200274ER



Photosynthetically-derived microalgae biomass is a promising alternative for the production of renewable alternatives to petroleum commodities. Usually, microalgal biomass production is focused on the carbon fraction, while the rest remain underutilized. The project aims to express cyanophycin (a polymer with potential industrial uses) as a way to increase value in the nitrogen-containing fraction. Since cyanophycin is produced from a different precursor pool than lipids and carbohydrates, the polymer can be co-produced within a cell, thus adding value and flexibility to microalgal biomanufacturing processes.

Project Description

Due to increasing global environmental and social pressures (global warming, depleting oil reserves and food scarcity) we must develop microbial-based systems for commodity chemical production. Photosynthetic platforms such as microalgae are desirable, because they can utilize carbon dioxide and sunlight to produce complex molecules. Lipids and carbohydrates from microalgae can be used to produce liquid biofuels; however, the protein fraction is generally underutilized. In order to use the protein fraction, we will engineer the production of cyanophycin into the microalga Picochlorum soloecismus. Cyanophycin is a water-insoluble biologically-produced polymer that can be used as precursor to biodegradable coatings and adsorbants. We will utilize our expertise in engineering cyanobacterial and microalgal strains to introduce a synthetic cyanophycin synthesis gene into microalage and assess the effects of cyanophycin production on overall metabolism. In addition, we will manipulate protein elements that regulate nutrient balance, to allow for the optimal and simultaneous production of cyanophycin (coatings/adsorbants precursor) and lipid (fuel precursor) production. Producing a nitrogen-based polymer, such as cyanophycin, in microalgae to co-accumulate with other carbon storage molecules, and demonstrating the capacity to regulate algae metabolism, is a new approach that will further advance renewable chemical production.

Technical Outcomes

The project met the goal of manipulating the biochemical composition of the microalga Picochlorum soloecismus by manipulating phosphorus concentration in growth media. Additionally, the implementation of ‘omic and analytical technologies on Pichochlorum’s cultures has provided with a deeper understanding of Phosphate-associated metabolic regulation, enabling future research in the field.

Publications

Journal Articles

Gonzalez Esquer, C. R., N. M. Sudasinghe, S. Negi, C. K. Sanders, S. L. Pacheco and T. T. Dale. Physiological response to phosphate depletion in the microalga Picochlorum soloecismus. Submitted to *Algal Research*. (LA-UR-22-30177)

Reports

Sudasinghe Appuhamilage, N. M. and A. Meek. Literature Review and Summary of Assays. Unpublished report. (LA-UR-22-28463)

Sudasinghe Appuhamilage, N. M. and A. Meek. Papers-Topics. Unpublished report. (LA-UR-22-28548)

Presentation Slides

Sudasinghe Appuhamilage, N. M. Algae Pigment Analysis. . (LA-UR-22-25540)

Dale, T. T. Biofuels and Biomanufacturing for the Arctic Energy Office. . (LA-UR-22-21990)

Posters

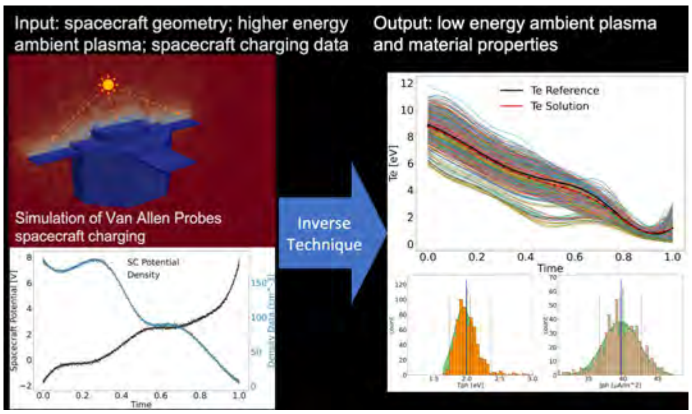
Gonzalez Esquer, C. R., S. Negi, T. S. Werner and T. T. Dale. Manipulating the biochemical composition in Picochlorum soloecismus for optimal nutrient fractionation into renewable chemicals. Presented at *International Conference on Algal Biomass, Biofuels and Bioproducts*, ONLINE, New Mexico, United States, 2021-06-14 - 2021-06-16. (LA-UR-21-25534)

Meek, A., N. M. Sudasinghe Appuhamilage, C. R. Gonzalez Esquer, T. T. Dale and S. Negi. Calculating Cyanophycin Production in Cyanobacteria. Presented at *2022 Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27929)

**Peer-reviewed*

Inverse Problem Approach to Spacecraft Charging Simulations

Gian Delzanno
20200276ER



Spacecraft orbiting the Earth become electrically charged by collecting plasma particles and by emitting electrons via secondary- and photo-emission. This is called spacecraft charging. Direct calculations of spacecraft charging require knowledge of the spacecraft materials and the ambient plasma. Unfortunately, the properties of the low-energy (~eV) ambient particles are typically not known and spacecraft material properties have big uncertainties due to degradation caused by the interaction with the space environment. To solve these problems, the project team developed an inverse approach to use available spacecraft charging data to infer the missing properties of the space environment near the spacecraft and material aging.

Project Description

Spacecraft (satellite) charging is a major application of space-weather research since charging can lead to spacecraft anomalies. The latter can range from inconsequential to catastrophic (damage to sensitive electronics and total loss of the spacecraft). Unfortunately, current direct spacecraft-charging calculations are extremely limited due to uncertainties in the space environment and material parameters (the latter degrade due to radiation damage during the spacecraft mission in space). To address this problem, we will develop for the first time an inverse approach to use available spacecraft-charging data to infer important information regarding the space environment around the spacecraft and material degradation. Our long-term goals are to (1) learn critical information about the space environment (in particular the low-energy particles, a key component of space-weather research), (2) understand how materials age in space (with important national-security applications), and (3) assist operators in the resolution of spacecraft anomalies.

Technical Outcomes

This project successfully developed an inversion technique for spacecraft surface charging calculations and validated it against datasets from the Van Allen Probes spacecraft. The technique was used to calculate some properties of the low-energy populations of the Earth's magnetosphere, helping develop a new understanding of these mysterious populations. Spacecraft-material photoemission properties were also obtained for several datasets, showing the utility of the technique for material-aging studies and its potential for spacecraft anomaly resolution.

Publications

Journal Articles

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Conference Papers

Resendiz Lira, P. A., G. L. Delzanno, H. C. Godinez Vazquez, M. G. Henderson, B. E. Wohlberg and D. Svyatsky. Inverse Problem Approach to Spacecraft Charging Simulations. Presented at *16th Spacecraft Charging Technology Conderence*. (Virtual, New Mexico, United States, 2022-04-04 - 2022-04-08). (LA-UR-22-25049)

Resendiz Lira, P. A., G. L. Delzanno, H. C. Godinez Vazquez, M. G. Henderson, D. Svyatsky and B. E. Wohlberg. Inverse Problem Approach to Spacecraft Charging Simulations. Presented at *16th Spacecraft Charging Technology Conference*. (Virtual, New Mexico, United States, 2022-04-04 - 2022-04-08). (LA-UR-22-24461)

Resendiz Lira, P. A., G. L. Delzanno, M. G. Henderson, H. C. Godinez Vazquez, B. E. Wohlberg and D. Svyatsky. Validation of an Inverse Technique for Spacecraft Charging Modeling with Van Allen Probes Data. Presented at *The 16th Spacecraft Charging Technology Conference*. (Virtual, New Mexico, United States, 2022-04-04 - 2022-04-08). (LA-UR-22-25048)

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Delzanno, G. L., J. E. Borovsky, J. Bortnik, C. R. Chappell, P. A. Fernandes, D. Gallagher, J. Goldstein, M. G. Henderson, J. C. Holmes, G. B. Hospodarsky, V. K. Jordanova, C. A. Maldonado, Y. Nishimura, D. B. Reisenfeld, V. Roytershteyn, R. M. Skoug, E. Spanswick, M. Usanova, E. Donovan, P. A. Resendiz Lira, O. Koshkarov and D. Svyatsky. The Need to Understand the Cold Ion and Cold Electron Populations of the Earth's Magnetosphere:. Unpublished report. (LA-UR-22-27269)

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Delzanno, G. L. Why can't we measure the hidden magnetosphere?. . (LA-UR-21-26008)

Delzanno, G. L. Spacecraft charging. . (LA-UR-21-26013)

Delzanno, G. L. How can we measure the hidden magnetosphere?. . (LA-UR-21-25987)

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Delzanno, G. L. The impact of the cold plasma in magnetospheric physics: Summary of initial discussions of strategies for Decadal Survey white papers. Presented at *VGEM*, Online, District Of Columbia, United States, 2021-07-29 - 2021-07-29. (LA-UR-21-27435)

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Resendiz Lira, P. A., G. L. Delzanno, M. G. Henderson, H. C. Godinez Vazquez, D. Svyatsky and B. E. Wohlberg. Validation of an Inverse Technique for Spacecraft Charging Modeling with Van Allen Probes Data. Presented at *The*

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Godinez Vazquez, H. C. Data Assimilation Methods for Dynamical Systems. . (LA-UR-21-26245)

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Godinez Vazquez, H. C. and M. G. Henderson. Data Assimilation for Radiation Belt Diffusion Coefficients using Adjoint Models. Presented at *Workshop on machine Learning, data Mining and data Assimilation in Geospace (LMAG2020)*, Online, New Mexico, United States, 2020-09-21 - 2020-09-25. (LA-UR-20-27392)

Posters

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Quinn, D. C., P. A. Resendiz Lira, M. G. Henderson and G. L. Delzanno. Properties of Cold Electrons in the Earth's Magnetosphere. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27928)

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**Peer-reviewed*

Nanotherapeutic Adjuvants for Sepsis

Jessica Kubicek-Sutherland
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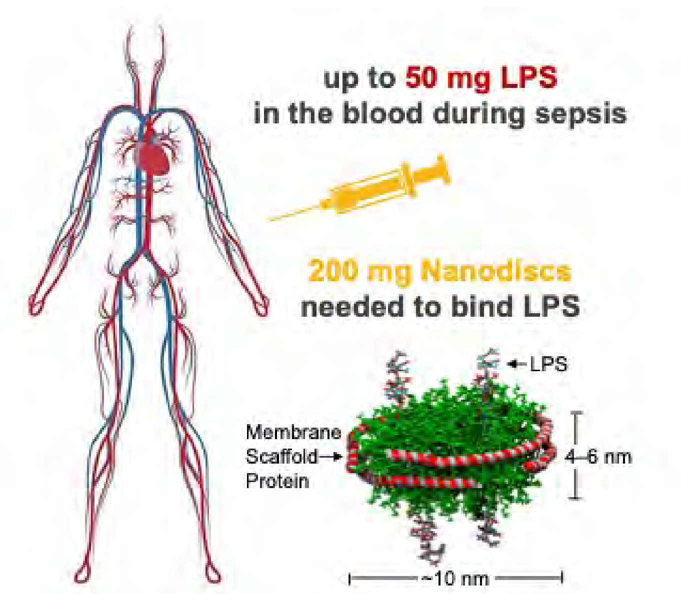

Sepsis is a leading cause of death with limited diagnostic and treatment options.Researcher at Los Alamos have developed a novel pipeline for the rational design and formulation of synthetic lipoproteins for use as sepsis therapeutics. These synthetic nanotherapeutics are broadly active and can be administered at the first indication of illness or injury in order to slow the disease progress and buy time for an accurate diagnosis and effective treatment to be started.

Project Description

Sepsis is a leading cause of death in children, the critically-ill, and warfighters. The lack of rapid and accurate diagnostics limits the utility of available therapeutics, which is a profound challenge in treating combat-related injuries where battlefield conditions further limit access to diagnostic and therapeutic resources. An adjuvant therapeutic strategy that delays the onset of severe sepsis in order to provide more time for the initiation of effective treatment could save countless lives. Sepsis occurs following an infection that leads to an overwhelming inflammatory response. The bacterial cell wall component lipopolysaccharide (LPS) is one of the most potent immune activators and causes of severe sepsis. Strategies that inhibit LPS activation of the immune system can provide adjunctive therapy that reduces the severity of symptoms and mortality associated with sepsis. Here, we will rationally design nanoparticles that specifically bind and sequester LPS in order to inhibit its toxicity. To do so we will combine theoretical modeling and simulation with experimental characterization to create novel nanotherapeutics for sepsis, which will also form the foundations for a pipeline to develop targeted nanotherapeutics for other molecules of interest on demand.

Technical Outcomes

This project successfully developed an integrated computational and experimental capability for generating lipoprotein nanodisc-based capture ligands that bind molecules of interest, starting with bacterial lipopolysaccharide (LPS). The high-throughput computational protocol screens nanodiscs with varying lipid and protein composition, and predicted a novel cationic nanodisc formulation that was verified by experiments to inhibit LPS toxicity. Incorporation of receptor proteins has further expanded the design of nanodisc-based capture molecules for both therapeutic and diagnostics applications.

Publications

Journal Articles

Lopez Bautista, C. A., P. A. Kocheril, M. I. Hiller, D. E. Jacobsen, K. E. Klosterman, K. D. Lenz, J. Z. Kubicek-Sutherland and S. Gnanakaran. Computationally-guided design of cationic-enriched lipid platforms for the capture of bacterial lipopolysaccharide. Submitted to *Nature Nanotechnology*. (LA-UR-21-31125)

Kocheril, P. A., L. A. Patel, J. G. Schmidt, K. D. Lenz, K. E. Klosterman, M. I. Hiller, S. Gnanakaran, H. Mukundan and J. Z. Kubicek-Sutherland. Phosphocholine nanodisc binds minimized atrial natriuretic peptide with high-nanomolar affinity. Submitted to *Journal of Physical Chemistry B*. (LA-UR-22-21060)

Kubicek-Sutherland, J. Z., P. A. Kocheril, M. I. Hiller, D. E. Jacobsen and K. D. Lenz. Comparability of high-density lipoprotein measurements by isothermal titration calorimetry. Submitted to *Analytical Biochemistry*. (LA-UR-21-31630)

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Stromberg, L., M. M. Jones, A. Bitzer, S. Courtney, S. Jakhar, S. C. Moore, K. E. Klosterman, M. I. Hiller, L. Lilley, Z. Stromberg, K. D. Lenz, J. Z. Kubicek-Sutherland and H. Mukundan. Understanding the Role of Amphiphilicity in Pathogen-Host Interactions during Innate Immunity: Gram-negative bacteria. Submitted to *Sage Journals*. (LA-UR-23-21975)

Stromberg, L., T. R. Llewellyn, M. M. Jones, A. Bitzer, S. Courtney, S. Jakhar, S. C. Moore, K. E. Klosterman, L. Lilley, Z. Stromberg, K. D. Lenz, J. Z. Kubicek-Sutherland and H. Mukundan. Understanding the Role of Amphiphilicity in Host-Pathogen Interactions During Innate Immunity: Gram-variable bacteria. Submitted to *Sage Journals*. (LA-UR-23-21970)

Books/Chapters

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Lopez Bautista, C. A. Formulation of lipid nanoplatforms for the treatment of bacterial sepsis. . (LA-UR-21-21426)

Lopez Bautista, C. A. Computational engineering of Human Apolipoprotein for enhanced interaction with bacterial toxins. . (LA-UR-22-20411)

Lopez Bautista, C. A. HIV Env assembling is tightly modulated by lipid composition and cytoplasmic tail integrity. . (LA-UR-22-27459)

Klosterman, K. E., K. D. Lenz, H. Mukundan and J. Z. Kubicek-Sutherland. BIOPHYSICAL CHARACTERIZATION OF HUMAN LIPOPROTEINS FOR DIAGNOSTIC ASSAY DEVELOPMENT. Presented at *Biophysical Society Annual Meeting 2021*, Virtual, New Mexico, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-20471)

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Posters

Hiller, M. I., K. D. Lenz, P. A. Kocheril, D. E. Jacobsen, C. A. Lopez Bautista, S. Gnanakaran and J. Z. Kubicek-Sutherland. Formulation and Screening of Synthetic Lipoproteins for Binding and Inhibition of Endotoxin.. Presented at *Biophysical Society Annual Meeting*, San Francisco, California, United States, 2022-02-19 - 2022-02-23. (LA-UR-22-20953)

Hiller, M. I., P. A. Kocheril, K. D. Lenz, D. E. Jacobsen, C. A. Lopez Bautista, S. Gnanakaran and J. Z. Kubicek-Sutherland. Synthetic host-mimics for sequestration of endotoxin. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27081)

Klosterman, K. E., K. D. Lenz, H. Mukundan and J. Z. Kubicek-Sutherland. BIOPHYSICAL CHARACTERIZATION OF HUMAN

LIPOPROTEINS FOR DIAGNOSTIC ASSAY DEVELOPMENT. Presented at *Biophysical Society Annual Meeting 2021*, Virtual, New Mexico, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-20305)

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Kubicek-Sutherland, J. Z., S. Jakhar, K. D. Lenz, D. E. Jacobsen, P. A. Kocheril, K. E. Klosterman and H. Mukundan. Serum lipoproteins and lipoarabinomannan suppress the inflammatory response induced by the mycolactone toxin. Presented at *ASM Microbe 2022*, Washington D.C., District Of Columbia, United States, 2022-06-09 - 2022-06-13. (LA-UR-22-24891)

**Peer-reviewed*

Particle Modeling of High-Altitude Nuclear Explosions

Ari Le

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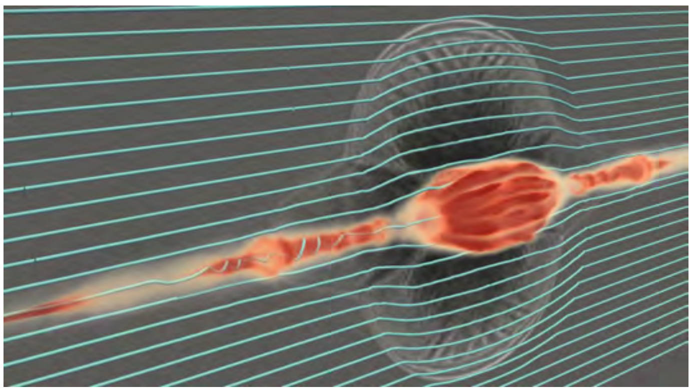

Detailed models of High-Altitude Nuclear Explosions (HANEs) including kinetic ions with the Hybrid VPIC code are enabling predictions about HANE debris transport across a wide range of parameters. The kinetic modeling is necessary to quantify the transport of HANE debris (orange) parallel to the geomagnetic field (cyan lines) and to capture kinetic coupling processes in the tenuous natural plasma above ~200 km altitude.

Project Description

High-Altitude Nuclear Explosions (HANEs) pose a threat to national security by generating a large-scale Electro-Magnetic Pulse (“blast” or “E3A” EMP) that could knock out large portions of the power grid by coupling to long-distance transmission lines, as well as by filling near-Earth space with beta radiation harmful to satellite technology. Current fluid models fail to accurately predict both of these processes because they miss key kinetic plasma physics that our project addresses. We will develop a hybrid (kinetic ion/fluid electron) code, and we will use it to explore unanswered basic questions about HANEs and E3A EMP generation: (1) How is radioactive debris transported to high altitudes? (2) What is the role of kinetic ion instabilities in generating local E3A EMP fields? And (3) how does HANE physics change at very high altitudes (> 800 km)? We will compare our model to historical HANE test data. Additional rigorous validation tests of the underlying plasma physics will be done with data from laboratory experiments and with spacecraft data from Earth’s magnetosphere.

Technical Outcomes

The project delivered a hybrid (kinetic ion/fluid electron) code suitable for modeling ionized debris transport from high-altitude nuclear explosions in the collisionless regime (above about 250 kilometer altitude). The code, Hybrid-Vector Particle-In-Cell (VPIC), was validated with laboratory and space data. The electromagnetic coupling between weapon debris and the ionosphere was studied, and details of the kinetic instabilities were published in open journals.

Publications

Journal Articles

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Le, A. Y., D. Winske, M. Cowee, A. J. Stanier, W. S. Daughton, C. Niemann, P. Heuer, R. Dorst and C. Constantin. Validating the new LANL 3-D hybrid HANE model with UCLA laser target experiment data. Submitted to *Journal of Radiation Effects, Research, and Engineering*. (LA-UR-20-23122)

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*Tang, B. -., W. Y. Li, D. B. Graham, C. Wang, Y. V. Khotyaintsev, A. Le, B. L. Giles, P. -. Lindqvist, R. E. Ergun and J. L. Burch. Lower Hybrid Waves at the Magnetosheath Separatrix Region. 2020. *Geophysical Research Letters*. **47** (20): e2020GL089880. (LA-UR-20-27264 DOI: 10.1029/2020GL089880)

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Blinov, S. D., N. M. Mackey, A. Y. Le and A. J. Stanier. Dynamics of Plasma Blobs in Curved Magnetic Geometries. . (LA-UR-22-28335)

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Le, A. Y. High-Altitude Nuclear Explosion Calculation performed on Grizzly for Institutional Computing Project w20_hybpasma. . (LA-UR-21-21809)

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Le, A. Y., D. Winske, M. Cowee, F. Guo, A. J. Stanier, W. S. Daughton, D. J. Stark and S. V. Luedtke. Update on HANE Modeling with Hybrid-VPIC. . (LA-UR-20-30045)

Le, A. Y., D. Winske, W. S. Daughton, M. Cowee, C. Niemann, P. Heuer, R. Dorst and C. Constantin. Validating the new LANL 3-D hybrid HANE code with UCLA laser data. Presented at *Hardened Electronics and Radiation Technology (HEART) 2020*, Louisville, Kentucky, United States, 2020-03-23 - 2020-03-23. (LA-CP-20-20105)

Le, A. Y., L. Yin, A. J. Stanier, B. A. Wetherton, B. Keenan, D. Winske, M. Cowee, F. Guo, Q. Zhang, S. V. Luedtke, W. S. Daughton, B. J. Albright, L. J. Chen, C. Forest, J. Egedal, D. Endrizzi, C. Dong and L. Wang. Hybrid-VPIC Code and Applications. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-17. (LA-UR-22-30756)

Le, A. Y., V. Roytershteyn, H. Karimabadi, A. J. Stanier, L. Chacon and K. Schneider. Wavelet Methods for Studying the Onset of Strong Plasma Turbulence. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New

Mexico, United States, 2020-03-09 - 2020-03-09. (LA-UR-20-21673)

Le, A. Y., W. S. Daughton, A. J. Stanier, L. J. Chen, S. Wang, J. Ng, J. Egedal, Y. H. Liu, W. D. Nystrom and R. F. Bird. Magnetic reconnection under the microscope: 3D PIC simulations of reconnecting current sheets. Presented at *U Wisconsin Plasma Physics Seminar*, Online, New Mexico, United States, 2020-10-19 - 2020-10-19. (LA-UR-20-28186)

Wetherton, B. A., A. Y. Le, C. Dong and L. Wang. Reconnection in hybrid global magnetosphere modeling of Mercury. Presented at *GEM Summer Workshop*, Honolulu, Hawaii, United States, 2022-06-20 - 2022-06-24. (LA-UR-22-25462)

Wetherton, B. A., J. Egedal, A. Y. Le and W. S. Daughton. Generation of a strong parallel electric field and embedded electron jet in the exhaust of moderate guide field reconnection. Presented at *Magnetic Reconnection Workshop 2022*, Monterey, California, United States, 2022-05-16 - 2022-05-20. (LA-UR-22-24135)

Wetherton, B. A., J. Egedal, A. Y. Le and W. S. Daughton. Generation of a strong parallel electric field and embedded electron jet in the exhaust of moderate guide field reconnection. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30379)

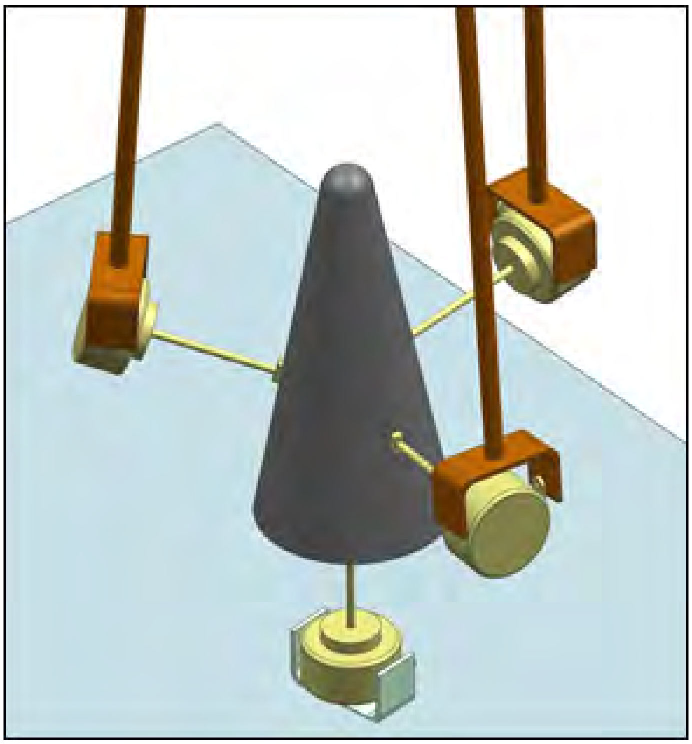
Posters

Wetherton, B. A., J. Egedal, P. K. Montag, A. Y. Le and W. S. Daughton. A Drift-Kinetic Method for Obtaining Gradients in Plasma Properties From Single-Point Distribution Function Data. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, Remote, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28931)

**Peer-reviewed*

Multi-axis Dynamic Modeling of Environmental Capture Re-entry Body Configuration

Thomas Sant
20210724ER



The project will create finite element analysis (FEA) model to simulate the enhanced fidelity instrumented mod A (EFI-A) flight test. This FEA will need to be capable of being driven by multiple inputs, not the standard single input of traditional FEAs. Model will be evaluated for its ability to recreate the flight environment for both the Re-entry Body (RB) exterior measured locations and internal measured locations.

Project Description

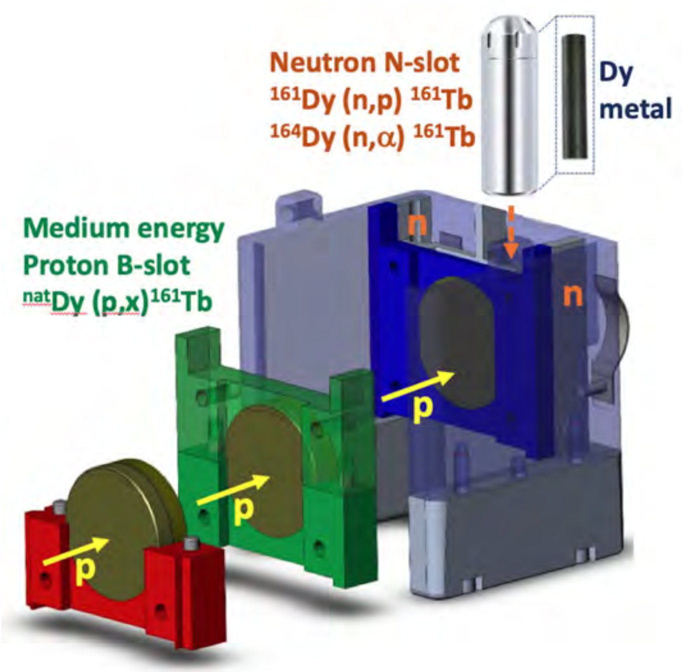
Department of Energy (DOE) and Department of Defense (DoD) agencies are already building capabilities and facilities to perform multi-axis shock and vibration testing with the intent to utilize them for future system qualification efforts. In order to understand the impacts of these types of tests on weapon systems and how the data from these tests should be used to inform physics components designs, Los Alamos National Laboratory (LANL) needs to build the capabilities to model these new types of testing.

Technical Outcomes

In alignment with the goal of simulating a high-fidelity Reentry Body in a multi-axis vibration environment, a structural dynamics workflow was developed to guide efforts in reduced-order modeling (ROM). A ROM algorithm and non-linear eigenvalue problem algorithm were also developed and shown to work well for a small number of components. The team expects the algorithms to scale well with the size of the structure and to be capable of accurate analysis of complicated structures.

Terbium-161 for Targeted Radionuclide Therapy

Veronika Mocko
20210842ER



Radioisotope production target stack at the Isotope Production Facility (IPF) at LANSCE indicating possible production pathways for the emerging therapeutic radionuclide Terbium-161. Two different accelerator-based pathways are being explored to produce Terbium-161 from natural dysprosium (1) proton induced reactions using medium energy protons (40-65 MeV) from the primary proton beam and (2) neutron-induced reactions utilizing the high-energy secondary neutron flux generated when the primary proton beam interacts with the IPF target stack. The second part of this project will focus on optimizing the separation of a small amount of terbium (micrograms) from a massive dysprosium target (mg - g).

Project Description

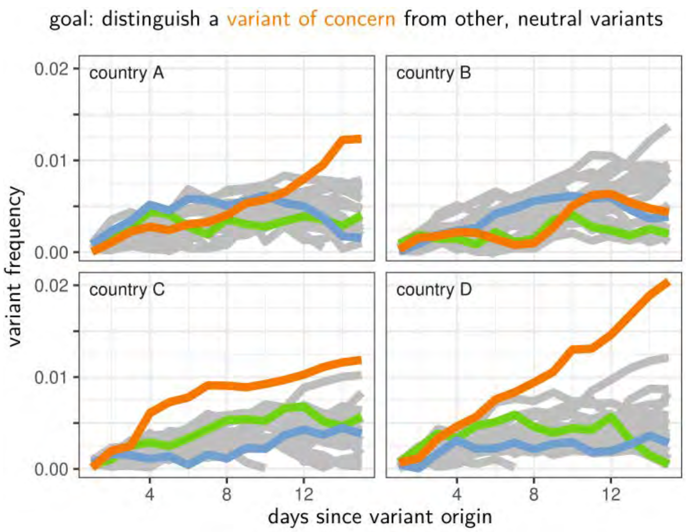
United States (US) domestic production of key radioactive and stable isotopes has significantly diminished, leaving patients and industry vulnerable to disruptions of our mostly foreign supply. New diagnostic and therapeutic agent development is needed to reduce US dependency on foreign supply and to ensure National Preparedness. Cancer is the second-most deadly chronic disease in the US and it is important to increase the diversity of tools available to clinicians to fight this disease by increasing the number and type of radioisotopes accessible for treatment. This research will evaluate new ways to access medically relevant therapeutic radioisotope Terbium-161 whose therapeutic efficacy is expected to exceed the current clinical standard, Food and Drug Administration (FDA) approved Lutetium-177.

Technical Outcomes

Dysprosium targets were fabricated and projected yields calculated for production of terbium (Tb-161) via neutron- and proton-induced reactions on dysprosium metal. Preliminary data acquired for neutron-induced reactions on dysprosium suggest that this pathway is not viable to produce large amounts of high-purity Tb-161. The project developed a method to successfully separate microgram quantities of terbium from dysprosium.

Identifying Viral Variants of Concern in a World of Noisy Evolution

Emma Goldberg
20210887ER



These (simulated) data show one pathogen genetic variant that is favored by selection (orange), compared with twenty others that are neutral (gray, plus two highlighted in blue and green). The project team is developing mathematical modeling techniques to distinguish variants of concern soon after their appearance.

Project Description

As the ongoing coronavirus (COVID-19) pandemic rages across the globe, we are seeing an increasing number of headlines about new genetic variants that are transmitted more rapidly or are less susceptible to vaccines. This project's goal is to develop an analytic approach that can rapidly report whether a new genetic variant is a cause for concern. The result will aid public health responses to the pandemic---both within this country and globally---because the best hope of containing and quashing concerning variants is identifying them as early as possible.

Technical Outcomes

This project successfully developed a new method that quantifies the advantage of emerging viral genetic variants. Applying this approach showed, from early data, the greater advantage of variant Alpha than of Beta or R.1, and then even more so of Delta and Omicron. The approach has substantial power because it is based on a mathematical model of evolution, and it is relatively robust because it assesses the consistency of a variant's emergence in multiple countries.

Publications

Journal Articles

*van Dorp, C. H., E. E. Goldberg, N. Hengartner, R. Ke and E. O. Romero-Severson. Estimating the strength of selection for new SARS-CoV-2 variants. 2021. *Nature Communications*. **12** (1): 7239. (LA-UR-21-31253 DOI: 10.1038/s41467-021-27369-3)

van Dorp, C., E. E. Goldberg, R. Ke, N. W. Hengartner and E. Romero-Severson. Global estimates of the fitness advantage of SARS-CoV-2 variant Omicron. Submitted to *Virus Evolution*. (LA-UR-22-25181)

van Dorp, C., E. Goldberg, R. Ke, N. Hengartner and E. Romero-Severson. Global estimates of the fitness advantage of SARS-CoV-2 variant Omicron. *Virus Evolution*. **8** (2): veac089. (LA-UR-22-29227 DOI: 10.1093/ve/veac089)

**Peer-reviewed*

Controlled Granularity of High-fidelity Epidemiological Models: Aggregation, Disaggregation, and Boundary Effects

Carrie Manore
20220655ER

This work is geared toward creating multi-scale, multi-model frameworks that can provide robust projections and forecast for disease spread with quantified uncertainty to inform decision making. In particular, the team will be working on quantifying the utility of using coarser-grain models to inform high-fidelity models to increase both efficiency and accuracy.

Project Description

The use of epidemiological models to inform decision-makers during the coronavirus (COVID-19) pandemic has highlighted both successes and limitations of such models. The questions policy-makers ask span a wide range of scales and the timescales on which these answers are needed can vary also. Our proposed work will be a link to connection with data and real-time response, much as weather and hurricane forecasting has done. We will use coarse-grain models to robustly inform high-fidelity models needed for response, using uncertainty quantification.

Technical Outcomes

The project team finished up work on connecting data to model (EpiGrid) prediction primarily using coronavirus (COVID-19) data to validate results of the coarse-grain models so that they can be compared to the high-fidelity models (such as EpiCast). The project will lead to better results for model accuracy and inform new proposals.

Ocean Waves Modeling for Polar and Coastal Regions

Erin Thomas
20220659ER

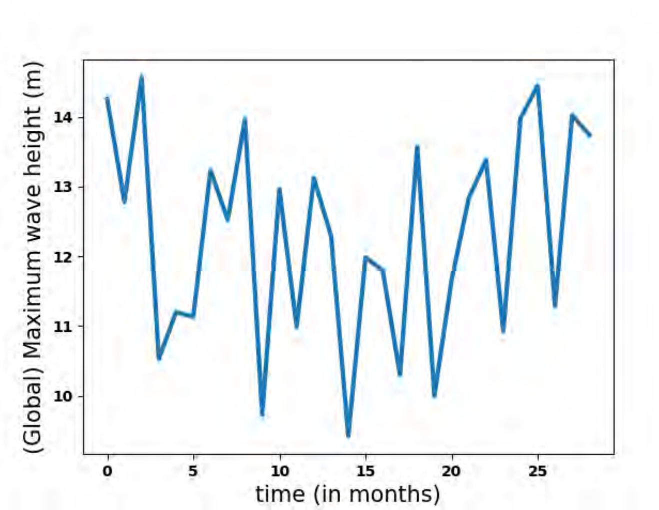


Image shows first results from WaveWatch 3 in E3SM coupled to the atmosphere for 28 months on a 100km uniform global unstructured mesh (courtesy of Nairita Pal, LANL, and Steven Brus, ANL).

Project Description

This project addresses a critical aspect of sea level rise associated with climate change, enabling ocean waves to be simulated in the Department of Energy's flagship climate model, Energy Exascale Earth System Model (E3SM), for predictions spanning at least the next fifty years, including interactions with sea ice along Arctic coasts, and attenuation of waves across the vast Southern Ocean sea ice pack. The work is necessary to help predict future frequency and severity of inundation events affecting the United States energy and national defense infrastructure, including at previous Pacific nuclear tests sites, and for understanding the impact on navigability of increasing wave activity in the Arctic under a depleting ice cover.

Technical Outcomes

This project identified optimal configuration of the existing WAVEWATCHIII software model for use within the Energy Exascale Earth System Model. The team determined large efficiency gains through reducing spectral resolution of the wave model and porting time-consuming wave source term calculations to graphic processing units. These modifications speed-up model runtime by 3x, allowing Los Alamos to produce cost efficient climate simulations containing the critical influence of ocean surface waves in the Arctic climate system.

Publications

Posters

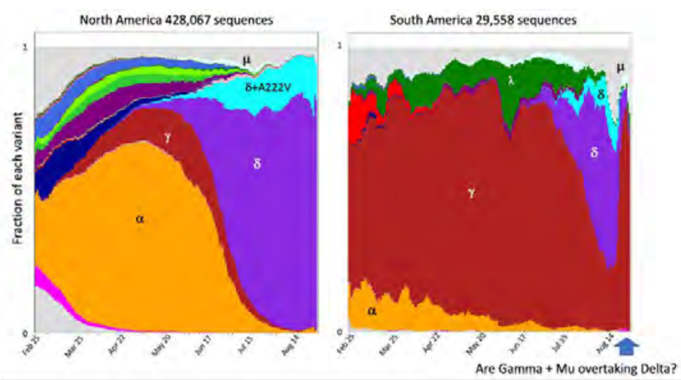
Ikuyajolu, O. J., L. Van Roekel, S. R. Brus, E. E. Thomas and Y. Deng. The impact of Wave state dependent fluxes on global climate in E3SMv2. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32690)

Thomas, E. E., S. Brus, O. Ikuyajolu and L. Van Roekel. WAVEWATCHIII Developments for Global Climate Simulations. Presented at *American Meteorological Society 17th Conference on Polar Meteorology and Oceanography*, Madison, Wisconsin, United States, 2022-08-08 - 2022-08-12. (LA-UR-22-27802)

**Peer-reviewed*

Epidemic Control and Viral Evolution, Coupling Epidemiology to Virology

Bette Korber
20220660ER



Weekly averages of the fraction of each major SARS-CoV-1 variant over the past 6 months. The Greek letters represent WHO variant designations. Delta is shown in purple, and a common Delta variant in turquoise. Alpha, originally from the UK, is shown in orange. Gamma, originally from Brazil, is shown in brick red. The forms of Gamma that are currently potentially competing favorable against Delta in South America contain additional infection-enhancing mutations relative to baseline Gamma. Sampling over the past few weeks is limited in South America and more data will be needed to confirm if this trend persists.

Project Description

The current Coronavirus Disease 2019 (COVID-19) pandemic poses considerable national public health and security challenges due to the economic and population impacts. Although vaccines were developed an unprecedented rate, the continuous mutation of Severe Acute Respiratory Syndrome-Coronavavirus 2 (SARS-CoV-2) presents additional new challenges. Thus, identifying newly emerging variants and their transmission characteristics is crucial for understanding and predicting their spread and best ways to mitigate their impact. The overarching goal of his project is to help focus scientific efforts on variants predicted to have the most potential to spread through bioinformatics and predictive modeling, and also inform response policy with a more accurate view of the epidemic potential of contemporary variants. Specifically, we will identify newly emerging variants, determine their transmission potential, and asses the vaccines' ability to protect against them. This information in turn will inform predictive epidemiological models that simulate and project the spread of competing variants across the United States, in the presence of heterogeneously vaccinated populations, and quantify the impact of different mitigation strategies to mitigate their spread.

Technical Outcomes

The critical outcome of this project was the development of a flexible framework to characterize variant transition dynamics through simple statistics that can applied across locations around the globe and identify possible factors contributing to their spread. Additionally the project team was able to apply sequencing analysis to the 2022 monkeypox outbreak.

Publications

Journal Articles

M. Korber, B. T., C. M. Gigante, J. P. Theiler, M. H. Seabolt, K. Wilkens, W. Davidson, A. Rao, H. Zhao, C. Hughes, F. Minhaj, M. Waltenburg, S. Smole, C. Brown, D. Blythe, R. Myers, J. Schulte, J. Stringer, P. Lee, D. Stanek, L. A. Griffin-Thomas, J. Crain, J. Murray, A. Adkinson, A. H. Gonalez, J. Nash, I. Daman, J. McQuiston, C. Hutson, A. McCollum and Y. Li. Multiple lineages of monkeypox virus detected in the United States, 2021- 2022. Submitted to *Science*. (LA-UR-22-30062)

M. Korber, B. T., S. Turner, W. M. Fischer, J. P. Theiler, H. Yoon and D. Smith. NIH/NIAID SAVE Early Detection Group: Prioritisation of SARS-VoC-2 Variants for Phenotyping and Horizon Scanning. Submitted to *Emerging Infectious Diseases*. (LA-UR-22-29260)

Moran, K. R. and S. Y. Del Valle. Insights gleaned from COVID-19 modelers and those they support. Submitted to *Nature*. (LA-UR-22-30789)

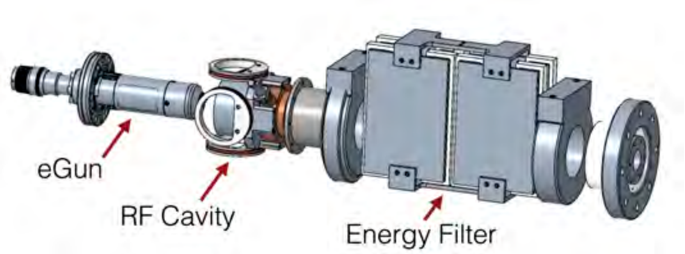
Presentation Slides

Castro, L. A. Forecasting COVID-19 Confirmed Cases and Deaths Across Geographic Scales: What went right, what went wrong, and the path to improvement. Presented at *BIRS Workshop on "Preparing for the Next Pandemic"*, Okanagan, Canada, 2022-06-13 - 2022-06-17. (LA-UR-22-25610)

**Peer-reviewed*

Laboratory Experiments Toward a Low Size, Weight, and Power (SWAP) Accelerator System for Space Applications

Edmond Reeves
20220664ER



A mechanical rendering of the three major sub-stems needed for an electron accelerator for use in space applications. In this configuration low size, weight, and power (SWAP) is achieved through use of a commercial electron gun, a single RF cavity driven by high electron mobility transformers (LANL patented) and a low-power, passive energy filter. The experimental testbed can be modified to test various components and complete systems.

Project Description

Electron beams in space have a number of potential national security applications. The most well-developed concept is to use them as "antennas" that generate very low frequency (very long wavelength) radio waves that are not practical for physical antennas. Those very low frequency (VLF) waves have possible communications applications but can also be used to remediate risks from natural or nuclear radiation belts by scattering radiation belt electrons. Charged particle beams (electrons or ions) are not practical for directed energy because charged particles cannot cross magnetic field lines. However charged particle beams are the initial technology needed for producing beams of neutral particles that can cross field lines and can therefore be used for directed energy applications. The same accelerator technology has been proposed for space propulsion systems. In those applications, charged particles the size of grains of sand can be accelerated to very high energies to produce thrust and function as a rocket engine. The advantage over conventional rocket engines is that the accelerator can operate on solar power and the particles that serve as "fuel" can be mined in space (e.g. from the Moon, Mars, or asteroids).

Technical Outcomes

Space-based accelerators have a number of potential applications. Electron beam ‘antennas’ have been proposed for radiation belt remediation; neutral beams have been proposed for directed energy applications; and nano-particle beams have been proposed for propulsion. In this project we designed and built a testbed where critical technologies and accelerator performance could be tested. This project developed and tested key parts of potential future space-based accelerator systems in a experimental laboratory environment.

Publications

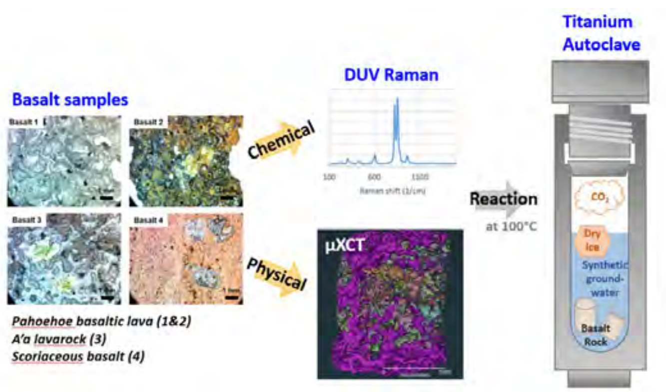
Posters

Roper, C. D., M. A. Holloway, A. S. Guider, D. E. Patrick, R. C. Clanton, E. G. D. Reeves, R. L. Hemphill, J. W. I. Lewellen, B. E. Carlsten, R. J. Aragonez, Q. R. Marksteiner and M. A. Mealy. The Beam Plasma Interactions Experiment (Beam-PIE): Progress on a sub-orbital active experiment using pulsed electron beams. Presented at *LANL 2022 Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-04. (LA-UR-22-28140)

**Peer-reviewed*

Promoting Carbon Dioxide (CO2) Mineralization During Geologic Carbon Sequestration in Mafic and Ultramafic Rocks

Chelsea Neil
20210640ECR



For the initial set of basalt reactivity experiments, four mineralogically-distinct basalt samples were characterized for their chemical compositions and physical traits (e.g., connected pore volume, porosity) before being reacted at 100°C in a series of titanium autoclaves, using dry ice to provide pressure and elevated CO2 concentrations. The goal of this set of experiments is to link basalt geochemical differences to their ability to mineralize CO2. Results will allow the team to recommend targeted basalt formation for geologic carbon sequestration in the field, and will provide experimental validation for reactive transport models being developed as part of this project.

Project Description

Storage of carbon dioxide (CO2) in subsurface geologic formations through geologic carbon sequestration (GCS) provides one of the best strategies for minimizing atmospheric CO2 emissions. Trapping of injected CO2 in this scenario relies heavily on the integrity of overlying, low permeability caprock, which has become a critical barrier to wider GCS implementation due to the inherent risk of CO2 leakage. Recent studies of GCS in mafic/ultramafic rock such as basalt have revealed mineralization thousands of times faster than that expected in other geologic formations, allowing for secure long-term CO2 storage as carbonate minerals. However, fast mineralization can be detrimental to long-term storage potential in these formations by quickly clogging pores and passivating reactive mineral surfaces. The goal of this project is to utilize integrated laboratory-scale experiments and newly developed pore-scale reactive transport models to evaluate interactions between injected CO2 and mafic/ultramafic rocks to identify conditions which promote mineralization and minimize detrimental impacts of fast precipitation. Through this work, we will provide critical new insights into the long-term safety and stability of stored CO2, as well as provide vital quantitative parameters needed to develop models that enable effective subsurface engineering and quantifying of risks associated with GCS in mafic/ultramafic rocks.

Publications

Journal Articles

Li, X., A. C. Jones, J. Choi, H. Zhao, V. Chandrasekaran, M. T. Pettes, A. Piryatinski, N. Sinitsyn, S. A. Crooker and H. Htoon. Proximity Induced Chiral Quantum Light Generation in Strain-Engineered WSe2/NiPS3 Heterostructures. Submitted to *Nature Nanotechnology*. (LA-UR-22-20519)

Neil, C. W., S. Li and C. D. Alcorn. In-situ Raman spectroscopic cell development for aqueous geochemistry at the solid-liquid interface. Submitted to *Review of Scientific Instruments*. (LA-UR-23-20897)

*Oglesby, S., S. A. Ivanov, A. Londono-Calderon, D. Pete, M. T. Pettes, A. C. Jones and S. Chabi. Manufacturing of Complex Silicon-Carbon Structures: Exploring SixCy Materials. 2022. *Materials*. **15** (10): 3475. (LA-UR-22-21434 DOI: 10.3390/ma15103475)

Schneider, M. E., H. L. Andrews, S. V. Baryshev, E. Jevarjian, D. Kim, K. Nichols, T. Y. Posos, M. T. Pettes, J. Power, J. Shao and E. I. Simakov. Effect of material composition of diamond field emission array cathodes on quality of transversely shaped beams. 2023. *Applied Physics Letters*. **122** (5): 054103. (LA-UR-23-21570 DOI: 10.1063/5.0128148)

Simakov, E. I., H. L. Andrews, S. Baryshev, E. Jevarijian, D. Kim, K. Nichols, T. Posos, M. T. Pettes, J. Power, J. Shao and M. E. Schneider. Evaluating Effects of Geometry and Material Composition on Production of Transversely Shaped Beams from Diamond Field Emission Array Cathodes. Submitted to *Journal of Applied Physics*. (LA-UR-22-30016)

Wang, X., M. T. Pettes, Y. Wang, J. Zhu, R. Dhall, C. Song, A. C. Jones, J. Ciston and J. Yoo. Edge states induced enhancement of exciton-to-trion conversion in proton irradiated WS2. Submitted to *Nature Communications*. (LA-UR-22-29441)

Wang, X., R. Kaufmann, R. Chen, T. Ahmed, M. T. Pettes, P. G. Kotula, I. Bilgin, S. Kar and J. Yoo. Nucleation of Hexagonal Germanium Grains on Defect Engineered Monolayer MoS2. Submitted to *Advanced Materials*. (LA-UR-22-23843)

Zhao, H., L. Zhu, X. Li, V. Chandrasekaran, J. K. S. Baldwin, M. T. Pettes, A. Piryatinski, L. Yang and H. Htoon. Manipulating Interlayer Excitons for Ultra-pure Quantum Light Generation. Submitted to *Nature Nanotechnology*. (LA-UR-22-23118)

Presentation Slides

Neil, C. W., D. J. Williams, M. T. Pettes, S. G. Young and B. M. Patterson. Natural basalt reactivity towards CO2: implications for geologic storage in mafic rocks. Presented at *Geological Society of America Annual Meeting*, Denver, Colorado, United States, 2022-10-09 - 2022-10-09. (LA-UR-22-29929)

Neil, C. W. and S. Li. Student Symposium Project Description. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-26160)

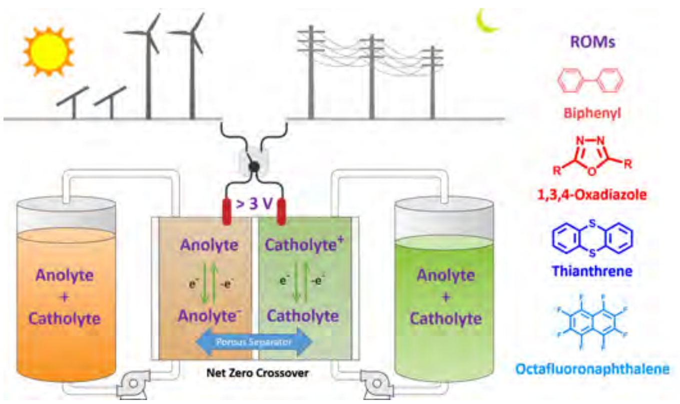
Neil, C. W. and S. Li. Designing a Pressure Cell for Geological Carbon Sequestration Studies. Presented at *2021 Summer Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27428)

Wu, H. and D. O'Malley. Physics embedded inverse analysis with automatic differentiation. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32627)

**Peer-reviewed*

Metal-free Redox-active Organic Molecules: A New Paradigm for Symmetric Non-aqueous Redox Flow Batteries

Sandipkumar Maurya
20210680ECR



The figure depicts the concept of mixed electrolyte-based symmetric redox flow batteries to be driven by functionalized redox-active organic molecules (ROMs). The derivatization of ROMs will enable non-aqueous flow battery operations > 3 V and at higher current densities due to improvement in ROMs solubility, redox potential, and reaction kinetics. The mixed electrolyte system can eliminate the need for a selective membrane and solve the inherent problems associated with active species crossover in non-aqueous redox flow batteries.

Project Description

A stable and reliable electricity grid is crucial to the United States economy and national security. The continuous addition of dynamic renewable energy sources into the Nation's electric grid jeopardizes the stability and reliability of the grid, potentially impacting national security. Batteries can provide crucial regulation to an electric grid predominantly fed by renewable energy. High-capacity batteries could provide electricity for minutes to hours, depending on their type. The current state of the art lithium-ion batteries are suitable for less than 4-hours operation; on the other hand, Vanadium redox flow batteries could run from a few hours to days. The cost analysis shows that more than 50% of the cost comes from the Vanadium raw material in the Redox flow batteries (RFB) system. Therefore, various Department of Energy (DOE) offices are continuously investing in next generation high capacity and power RFBs to replace vanadium with lower cost redox-active organic molecules. This project aims to achieve the ultimate cost target of $100 per kilowatt-hour (kWh) set by the Office of Electricity by developing low-cost, high capacity RFBs for integration into the Nation’s electric grid.

Publications

Journal Articles

Maurya, S., S. Diaz Abad, E. J. Park, K. Ramaiyan, Y. S. Kim, B. L. Davis and R. Mukundan. Phosphoric acid pre-treatment to tailor polybenzimidazole membranes for vanadium redox flow batteries. 2023. *Journal of Membrane Science*. **668**: 121233. (LA-UR-22-28889 DOI: 10.1016/j.memsci.2022.121233)

Presentation Slides

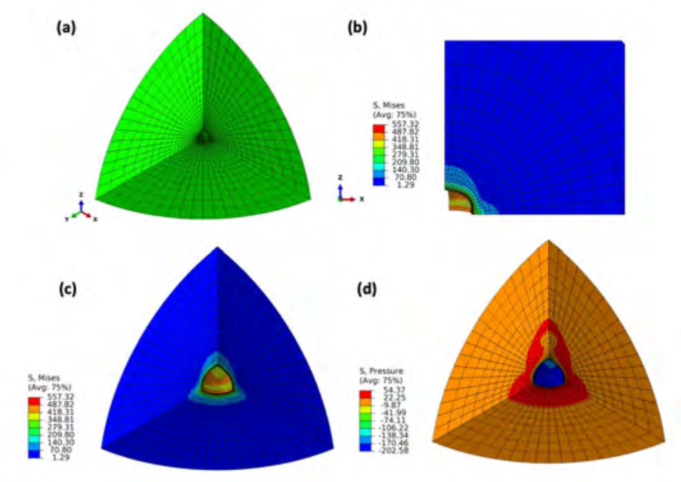
Maurya, S. Challenges and prospects of redox flow batteries: an overview of LANL activities. . (LA-UR-22-32177)

Maurya, S., T. Stracensky, A. B. Sweeney, K. A. Jesse, S. Diaz Abad, R. Mukundan and S. Mukerjee. Novel anolyte redox active organic molecules for redox flow battery applications. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30246)

**Peer-reviewed*

A Multiphysics Energy Approach to Modeling the Earth's Response to Underground Explosions

Kane Bennett
20210686ECR



Multiphysics material models implemented in finite element analysis capture the large irrecoverable (inelastic) deformation near the source and associated dissipation of energy in the ground due to underground explosions. New thermodynamically consistent large-deformation material modeling theory enables prediction of ground physical response mechanisms transitioning with distance from the source, enabling next generation of underground explosion modeling and simulation predictive capability: (a) initial mesh of 1/8 of sphere (taking advantage of symmetry) showing cavern wall at center; (b) expanded cavern after explosive loading, non-symmetric due to large-deformation anisotropy; (c) and (d) residual Mises stress and pressure (so-called "stress-cage confinement").

Project Description

A central challenge in seismic monitoring of underground nuclear explosions is discerning the energy yield of the source from seismic signal measurements obtained at large distances away (far-field measurements). Complex responses of the earth to the shock near the source (near-field), including melting, damage, plasticity, and the effects of fluid permeating the pore spaces of rock, greatly affect the propagation of the shock wave (signal) into the far-field, where the earth response eventually becomes elastic at some radius away. This project will provide new capability for modeling and simulation of the complex multiphysics response of the Earth to underground explosions. The interaction and feedbacks between the physical phenomena occurring in the near-field will be linked within a novel thermodynamically consistent framework, enabling simulations to provide the link between source yield and seismic signal measurements by resolving the dissipation of energy and resulting propagation of seismic signals near to the source.

Publications

Journal Articles

Bryant, E. C., N. A. Miller and K. Bennett. Data-driven modeling of granular matter's micro-macro dilation mismatch by volume constraint. Submitted to *Computers and Geotechnics*. (LA-UR-22-26740)

Wang, K., C. W. Johnson, K. C. Bennett and P. A. Johnson. Predicting Future Laboratory Fault Friction Through Deep Learning Transformer Models. 2022. *Geophysical Research Letters*. **49** (19): e2022GL098233. (LA-UR-22-20930 DOI: https://doi.org/10.1029/2022GL098233)

*Wang, K., C. W. Johnson, K. C. Bennett and P. A. Johnson. Predicting fault slip via transfer learning. 2021. *Nature Communications*. **12** (1): 7319. (LA-UR-21-26470 DOI: 10.1038/s41467-021-27553-5)

Reports

Stahl, A. M., K. Bennett and E. Rougier. Probing the effect of material model and geometry assumptions on ground response in the simulation of underground explosions. Unpublished report. (LA-UR-22-22336)

Presentation Slides

Bennett, K. and A. M. Stahl. A Multiphysics Energy Approach to Modeling the Earth's Response to Underground Explosions. Presented at *Internal open seminar*, Los Alamos, New Mexico, United States, 2022-07-11 - 2022-07-11. (LA-UR-22-26586)

Bryant, E. C., N. A. Miller and K. Bennett. Volume-Constrained Micromorphic Homogenization of Viscoelastic Viscoplasticity in Viscous-Binder-Bonded Particulate Materials. Presented at *MACH Conference*, Towson, Maryland, United States, 2023-04-05 - 2023-04-07. (LA-UR-23-22906)

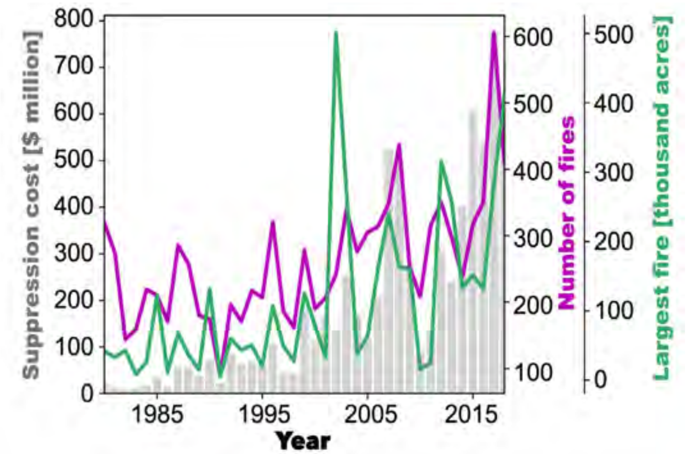
Posters

Stahl, A. M., K. Bennett and E. Rougier. Probing the Effect of Material Model and Geometry Assumptions in the Simulation of Underground Explosions. Presented at *56th U.S. Rock Mechanics Geomechanics Symposium*, Santa Fe, New Mexico, United States, 2022-06-26 - 2022-06-29. (LA-UR-22-25903)

**Peer-reviewed*

What Are the Main Drivers of Current Trends in Western Wildfires?

Alexandra Jonko
20210689ECR



The frequency, size, and suppression cost of wildfires in the State of California have all increased significantly over the past decades. Open questions remain about what causes these trends. LANL will use state-of-the-art modeling to improve our scientific understanding of how climate change, past forest management practices, and a rise in human-caused ignitions of wildfires play together to explain the recent uptick in wildfire activity in California. [Data source: fire.ca.gov]

Project Description

Wildfires in the western United States are dramatically increasing in frequency and severity, and the impacts on society are devastating: fatalities, economic costs, and loss of critical infrastructure. In just the last three years, California has experienced its largest wildfire, which burned over 800,000 acres (2020 August Complex), and its most deadly event, which resulted in 85 deaths (2018 Camp Fire). However, it remains unknown to what extent the recent devastating events are driven by the effects of (1) climate change, (2) a long history of fuel management based on fire suppression which has led to a build-up of fuels, or (3) an expansion of the wildland-urban interface and associated changes in how frequently wildfires are started by humans. These questions must be resolved to effectively prepare for future wildfire containment, infrastructure security, and land and water management. This project will establish hypothesis-tested scientific understanding of how compounding climate extremes, fuel management history, and changes in ignition sources tied to population density impact current wildfire trends in California, including larger burned area, increasing damage, and longer fire seasons, ultimately supporting decision-making for national security.

Publications

Journal Articles

Dickman, L. T., A. Jonko, R. R. Linn, I. Altintas, A. L. Atchley, A. B\xc3\xa4r, A. D. Collins, J. L. Dupuy, M. R. Gallagher, J. K. Hiers, C. M. Hoffman, S. Hood, M. D. Hurteau, W. M. Jolly, A. J. Josephson, E. L. Loudermilk, W. Ma, S. T. Michaletz, R. H. Nolan, J. O'Brien, R. Parsons, R. Partelli-Feltrin, F. Pimont, V. Resco de Dios, J. Restaino, K. A. Sartor, E. S. Schultz-Fellenz, S. P. Serbin, J. K. Shuman, C. Sieg, N. S. Skowronski, D. R. Weise, M. Wright, C. Xu, M. Yebra, N. Younes, S. A. Sevanto and Z. J. Robbins. Integrating plant physiology into simulation of fire behavior and effects. 2023. *New Phytologist*. (LA-UR-22-20430 DOI: 10.1111/nph.18770)

Jonko, A., J. A. Oliveto, T. M. Beaty, A. L. Atchley, J. Cronan, M. Dickinson, M. Gallagher, J. Kupfer, K. Hiers, C. Hoffman, M. Norris, M. North, R. Parsons, J. Restaino, C. Sieg, N. Skowronski, C. Teske, K. Williams and K. Yedinak. How will future climate change impact prescribed fire across the U.S.?. Submitted to *Nature Climate Change*. (LA-UR-22-30261)

McDanold, J. S., R. R. Linn, A. Jonko, A. L. Atchley, S. Goodrick, J. Hiers, C. M. Hoffman, E. Loudermilk, J. O'Brien, R. Parsons and C. Sieg. DUET - Distribution of Understory using Elliptical Transport: A mechanistic model of leaf litter and herbaceous spatial distribution based on tree canopy structure. Submitted to *Environmental Modelling & Software*. (LA-UR-22-24683)

Robbins, Z. J., C. Xu, A. Jonko, R. Chitra-Tarak, C. J. Fettig, J. Constanza, L. Mortenson, B. H. Aukema, L. M. Kueppers and R. M. Scheller. Carbon Stored in Live Ponderosa Pines in the Sierra Nevada Will Not Return toPre-drought (2012) Levels During the 21st Century Due to Bark Beetle Outbreaks.. Submitted to *Frontiers in Environmental Science*. (LA-UR-23-20308)

*Zhai, L., D. R. Coyle, D. Li and A. Jonko. Fire, insect and disease-caused tree mortalities increased in forests of greater structural diversity during drought. 2021. *Journal of Ecology*. **110** (3): 673-685. (LA-UR-21-28195 DOI: 10.1111/1365-2745.13830)

Presentation Slides

Jonko, A. Advancing coupled fire-atmosphere research with HIGRAD/FIRETEC (w20_firetec) - 2021 Institutional Computing Annual Progress Report. . (LA-UR-22-21864)

Jonko, A., J. A. Oliveto, T. M. Beaty and A. L. Atchley. How will future climate change impact prescribed fire across the US?. . (LA-UR-23-22630)

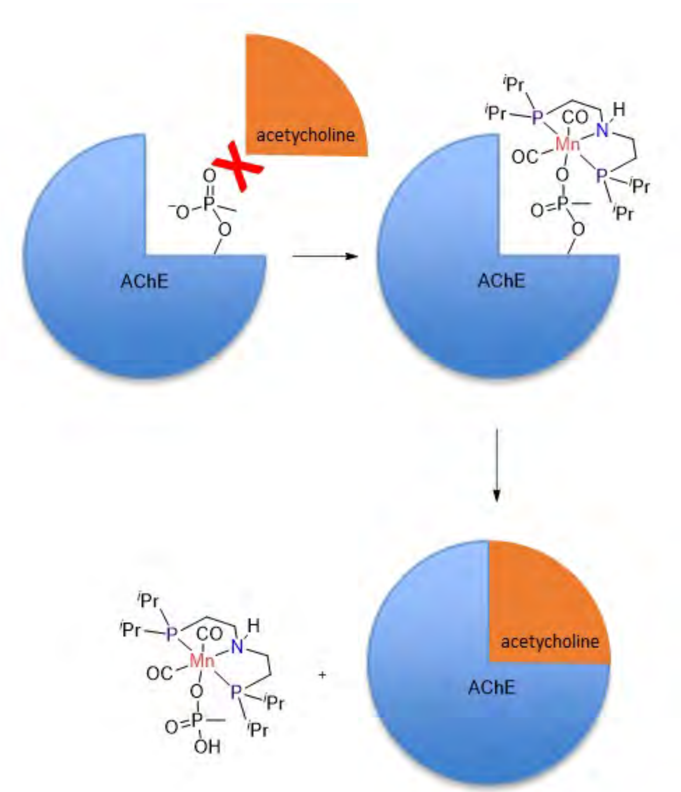
Posters

Robbins, Z. J., C. Xu, R. Chitra-Tarak, X. Gao, D. C. Koven, L. M. Kueppers, P. Boutte and A. Jonko. Quantifying chaparral-grassland competition across a fire and climatic gradient In Southern California, U.S.. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-16 - 2022-12-17. (LA-UR-22-32626)

**Peer-reviewed*

Inorganic Solutions to Organic Problems: Development of Transition Metal Based Acetylcholinesterase Reactivators

Brennan Billow
20220540ECR



Organophosphorus nerve agents effectively block the action of the essential acetylcholinesterase enzyme. Without acetylcholinesterase, the human body cannot function. The transition metal therapeutics, shown in the figure as a manganese based molecule, will remove the nerve agent from the active site of the enzyme, thus reactivating the enzyme and restoring normal bodily function.

Project Description

Nerve agents are a class of chemical weapon that have been exploited in a variety of political assassinations, terrorist attacks, and warfare. Our current medical countermeasures to treat nerve agent exposure victims rely on extremely dated methods. This project will lay the foundation for a new class of therapeutic to treat victims of nerve agent attacks. Specifically, we plan to develop of new class of therapeutic molecule based on transition metal elements. These elements are gaining popularity in a variety of medical fields and can be specifically tailored to meet the challenges faced by nerve agent poisonings. Through the course of this project we will demonstrate proof of concept therapeutic behavior of transition metal molecules and lay the groundwork for a paradigm shift in nerve agent exposure treatment.

Publications

Journal Articles

Livesay, B. N., J. G. Schmidt, R. F. Williams, B. S. Billow and A. Tondreau. Reactivity of [(PNP)Mn(CO)2] with Organophosphates. Submitted to *JACS Au*. (LA-UR-22-31194)

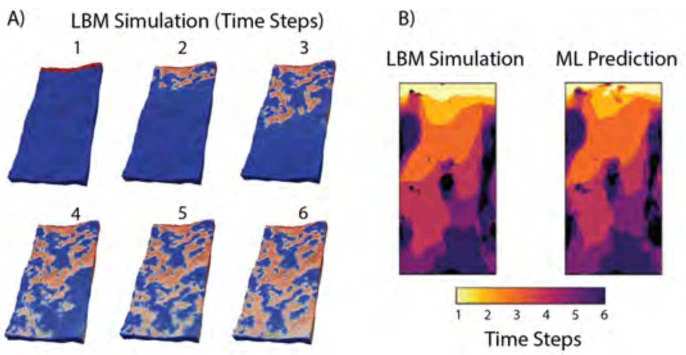
Posters

Livesay, B. N., B. S. Billow, J. G. Schmidt, R. F. Williams and A. Tondreau. Phosphorus-Fluorine Bond Hydrolysis Catalyzed by Transition Metal Complexes. Presented at *Gordon Research Conference (GRC) - Inorganic Chemistry*, Newport, Rhode Island, United States, 2022-05-28 - 2022-06-03. (LA-UR-22-25025)

**Peer-reviewed*

Multiphase Flow in Complex Fractures: Integrating Experimental Observations and Pore-Scale Models with Machine Learning

Eric Guiltinan
20220616ECR



This project aims to use machine learning to accelerate porescale simulations of multiphase fluid flow in fractures. A) Porescale simulation of carbon dioxide (red) displacing brine (blue) in a fracture. These simulations are computationally expensive requiring thousands of processors on the high performance computing cluster. B) Another porescale simulation with each time step overlapped and a machine learning simulation of the same fracture. Once trained, the machine learning simulation was completed in a fraction of a second on a conventional laptop.

Project Description

This work will address our ability to predict how fluids flow through fractures which has application to many Department of Energy/National Nuclear Security Administration mission areas. This work will allow for a better understanding of how contamination from nuclear waste might flow near a nuclear waste repository. It will also reduce uncertainties around carbon geologic storage and oil and gas production. Finally, this work will help predict gas migration from underground nuclear tests which will help with monitoring and verification.

Publications

Journal Articles

*Santos, J. E., A. Gigliotti, A. Bihani, C. Landry, M. A. Hesse, M. J. Pyrcz and M. Prodanovi\xc4\x87. MPLBM-UT: Multiphase LBM library for permeable media analysis. 2022. *SoftwareX*. **18**: 101097. (LA-UR-22-23120 DOI: 10.1016/j.softx.2022.101097)

Ting, A., J. A. Estrada Santos and E. J. Guiltinan. Learning Multiphase Flow through Complex Fractures. Submitted to *Energies*. (LA-UR-22-30110)

Conference Papers

Estrada Santos, J. A., D. O'Malley, M. Z. S. Mehana, H. S. Viswanathan and E. J. Guiltinan. Upscaling Microscale Flow Effects using Differential Programming. Presented at *CouFrac*. (Berkeley, California, United States, 2022-11-14 - 2022-11-14). (LA-UR-22-28612)

Welch, N. J., S. K. Peterson, J. A. Estrada Santos and E. J. Guiltinan. Multiphase flow experiments through 3D printed fractures. Presented at *3rd International Conference on Coupled Processes in Fractured Geological Media*. (Berkeley, California, United States, 2022-11-14 - 2022-11-14). (LA-UR-22-28683)

Reports

Ting, A., J. A. Estrada Santos and E. J. Guiltinan. Learning Multiphase Flow through Complex Fractures. Unpublished report. (LA-UR-22-28401)

Presentation Slides

Guiltinan, E. J. and B. Chen. Clean Hydrogen Production, Storage, Transport and Utilization to Enable a Net Zero Carbon Economy. . (LA-UR-22-29023)

Posters

Estrada Santos, J. A., D. O'Malley, M. Z. S. Mehana, H. S. Viswanathan and E. J. Guiltinan. Upscaling Microscale Flow Effects using Differential Programming. Presented at *CouFrac*, Berkeley, California, United States, 2022-11-14 - 2022-11-16. (LA-UR-22-31931)

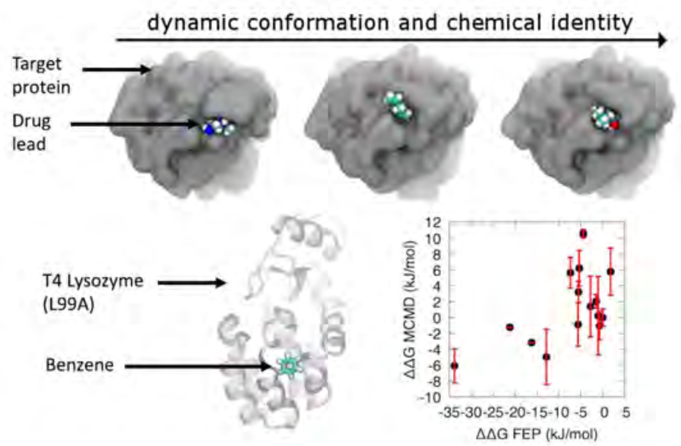
Ting, A. Forecasting Multiphase Flow through Fractures with Convolutional Neural Networks. . (LA-UR-22-27829)

Welch, N. J., S. K. Peterson, J. A. Estrada Santos, L. A. Chavez Atayde and E. J. Guiltinan. Multiphase flow experiments through 3D printed fractures. Presented at *Coufrac*, Berkeley, California, United States, 2022-11-14 - 2022-11-16. (LA-UR-22-31935)

**Peer-reviewed*

Drug Discovery by Automated Adaptation of Chemical Structure and Identity

Christopher Neale
20200543ECR



Existing drug discovery approaches are either fast or accurate, but not both. The team has developed a new Monte Carlo (MC)/molecular dynamics (MD) approach to drug discovery in which MC enables a chemical search and accounts for binding entropy while MD provides molecular flexibility and allows for induced-fit binding interactions. Application to cancer-causing Mutant Ras proteins provides new hypothesis, while testing on T4 lysozyme shows that the approach can rank-order compounds for a well-studied model system.

Project Description

New drugs require enormous capital investment. Our long-term goal is to dramatically reduce the total cost associated with bringing a drug to market. We are developing a new computational framework in which automated modifications to chemical formulas build upon previously accepted modifications so as to reward conceptually funnel-shaped regions comprising many chemicals that exhibit the desired properties (here, tight binding of the drug to the target protein). By directing the theoretical search toward chemical neighborhoods, rather than discrete chemicals, our approach will increase flexibility in subsequent attempts at lead refinement, thereby reducing the likelihood that drug candidates will succumb to late-stage failures. By design, this computational framework is also capable of guiding protein modifications for greater thermal stability (e.g., clean energy innovation via industrial carbon dioxide sequestration) and protein re-purposing for binding to exogenous compounds (e.g., toxins and biological agents), enabling toxin sequestration and signature detection with possible avenues for forward deployment via transgenic plants.

Technical Outcomes

The project developed a new computational method to rapidly design medical countermeasures. The method was implemented on high performance computing resources, and validated by comparison to existing approaches. This new method is applicable to the development of new drugs to counteract potential bioweapons, and to the re-engineering of proteins to detect or sequester toxins.

Publications

Journal Articles

Patel, L. A., P. N. U. Chau, S. G. Debesai, L. J. Darwin and C. A. Neale. Drug Discovery by Automated Adaptation of Chemical Structure and Identity. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-32243)

Patel, L. A., T. J. Waybright, A. G. Stephen and C. A. Neale. GAP Positions Catalytic H-Ras Residue Q61 for GTP Hydrolysis in Molecular Dynamics Simulations. Submitted to *Biophysical Journal*. (LA-UR-21-32240)

Wang, X., S. Kim, C. A. Neale, H. M. Warnakulasurya, J. Xu, P. Zhao, B. Kobilka, W. A. Goddard and L. Ye. Sequential Interhelical Molecular Switches Propagate Conformational Allostery for G Protein-coupled Receptor Activation. Submitted to *Nature*. (LA-UR-22-25183)

Reports

Neale, C. A., P. N. U. Chau, S. G. Debesai, L. J. Darwin and L. A. Patel. Drug Discovery by Automated Adaptation of Chemical Structure and Identity. Unpublished report. (LA-UR-22-22090)

Posters

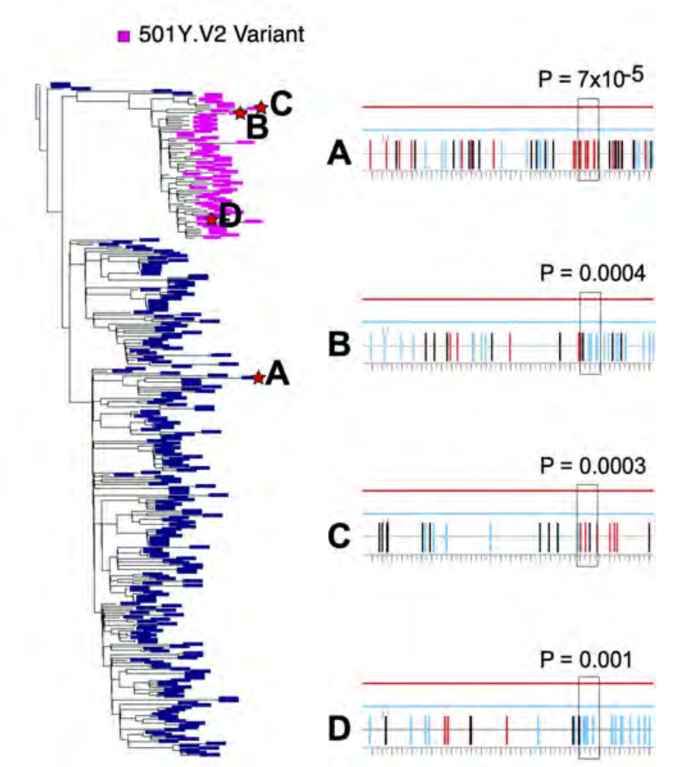
Debesai, S. G., L. A. Patel and C. A. Neale. Towards identifying drug candidates targeting oncogenic K-Ras via novel computational method. Presented at *Ras Initiative Symposium*, Silver Spring, Maryland, United States, 2021-05-24 - 2021-05-26. (LA-UR-21-24357)

Patel, L. A., C. A. Neale, T. J. Waybright and A. G. Stephen. GAP Positions Catalytic H-Ras Residue Q61 for GTP Hydrolysis in Simulations. Presented at *Ras Symposium*, Frederick, Maryland, United States, 2021-05-24 - 2021-05-26. (LA-UR-21-24328)

**Peer-reviewed*

Studying Recombination in Ribonucleic Acid Viruses and its Implications for Outbreak Surveillance and Health Interventions

Elena Giorgi
20200554ECR



This project aims to investigate the role of recombination in the evolution and spread of RNA viruses. While common in coronaviruses, identifying SARS-CoV-2 recombinants has been challenging due to the virus's initial homogeneity. Here we show 4 recombinants (A-D) identified among SARS-CoV-2 sequences sampled in South Africa at the time the new South African variant (501Y.V2) was starting to emerge (magenta in the phylogenetic tree on the left). Recombinants are shown as red stars on the tree on the left and the full genomes are shown in the panels on the left: parental strains are shown in red/blue solid lines and the recombinant carries blue/red mutations according to which parent it matches, black if it matches none.

Project Description

Human Immunodeficiency Virus 1 (HIV-1), Dengue, and Ebola are among the ten threats to global health in 2019 listed by the World Health Organization that "have potential to cause a public health emergency but lack effective treatments and vaccines." These highly infectious and often fatal viruses present a global health challenge due to their great genetic diversity, which can result in the rapid emergence of drug resistance and new outbreaks. Recombination—the rise of new viral strains from two genetically distinct parental viruses—is one of the molecular mechanisms that allow some viruses to rapidly diversify and acquire new traits, like increased virulence or drug resistance. While recombination occurs in many ribonucleic acid (RNA) viruses, its extent, rates, and role in selecting particular phenotypes are still open questions. Recombinants from animal reservoirs are particularly threatening as they have the potential to acquire greater virulence and to re-infect even previously exposed hosts. Recombinants also need to be accounted for when planning health interventions to either cure or prevent new infections as these viruses often have newly acquired drug and/or antibody resistance compared to non-recombinant viruses. This project will improve understanding of dangerous recombinants, leading to better outbreak predictions and medical interventions.

Technical Outcomes

The project demonstrated cross-species origin of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) through an evolutionary recombination event between bat and pangolin coronaviruses. Recombination was an important part of coronavirus evolution and common in wild bats. Additionally identified first recombinants within the SARS-CoV-2 pandemic and tracked evolution as new variants arose. In Human Immunodeficiency Virus (HIV), established the role of recombination in evolution of antibody resistant mutation and resistant-conferring changes in the envelope glycan shield.

Publications

Journal Articles

*G. E. E. *. C. S. *. N. K. *. B. T. *. T. J. *. G. P. A. *. Y. H. *. A. W. *. F. B. T. *. T. H. *. S. J. E. *. d. O. T. *. G. S. *. K. B. Fischer, W. *., E. E. Giorgi, S. Chakraborty, T. Bhattacharya, H. Yoon, B. T. Foley, S. Gnanakaran, W. Fischer, K. Nguyen, J. Theiler, W. Abfalterer and B. Korber. HIV-1 and SARS-CoV-2: Patterns in the evolution of two pandemic pathogens. 2021. *Cell Host & Microbe*. **29** (7): 1093-1110. (LA-UR-21-23163 DOI: 10.1016/j.chom.2021.05.012)

Giorgi, E. E., B. T. M. Korber, T. Bhattacharya, W. M. Fischer, W. P. Abfalterer and H. Yoon. Matters Arising response to: No evidence for increased transmissibility from recurrent mutations in SARS-CoV-2. Submitted to *Nature Communications*. (LA-UR-21-20393)

Giorgi, E. E., M. Honnayakanahalli Marichannegowda, J. T. Tu, D. R. Martinez, X. Li, L. Feng, S. R. Permar and F. Gao. Different evolutionary pathways of HIV-1 between fetus and mother perinatal transmission pairs indicate unique immune selection pressure in fetuses. Submitted to *Cell Reports Medicine*. (LA-UR-20-28189)

M. Korber, B. T., K. Wagh, E. E. Giorgi, B. Julg, M. S. Seaman, D. H. Barouch, G. D. Tomaras and A. deCamp. Rapid viral escape during triple broadly neutralizing monoclonal antibody therapy against HIV-1. Submitted to *Nature Medicine*. (LA-UR-21-25866)

*Korber, B., W. M. Fischer, S. Gnanakaran, H. Yoon, J. Theiler, W. Abfalterer, N. Hengartner, E. E. Giorgi, T. Bhattacharya, B. Foley, K. M. Hastie, M. D. Parker, D. G. Partridge, C. M. Evans, T. M. Freeman, T. I. de Silva, A. Angyal, R. L. Brown, L. Carrilero, L. R. Green, D. C. Groves, K. J. Johnson, A. J. Keeley, B. B. Lindsey, P. J. Parsons, M. Raza, S. Rowland-Jones, N. Smith, R. M. Tucker, D. Wang, M. D. Wyles, C. McDanal, L. G. Perez, H. Tang, A. Moon-Walker, S. P. Whelan, C. C. LaBranche, E. O. Saphire and D. C. Montefiori. Tracking Changes in SARS-CoV-2 Spike: Evidence that D614G Increases Infectivity of the COVID-19 Virus. 2020. *Cell*. **182** (4): 812-827. (LA-UR-20-23199 DOI: 10.1016/j.cell.2020.06.043)

*Li, X., E. E. Giorgi, M. H. Marichann, B. Foley, C. Xiao, X. Kong, Y. Chen, B. Korber, F. Gao and S. Gnanakaran. Emergence of SARS-CoV-2 through recombination and strong purifying selection. 2020. *Science Advances*. **6** (27): eabb9153. (LA-UR-20-22544 DOI: 10.1126/sciadv.abb9153)

Presentation Slides

Bhattacharya, T. Studying Viral Change in HIV and Coronavirus. . (LA-UR-20-25180)

Giorgi, E. E., K. Wagh, P. T. Hraber, B. T. M. Korber, G. M. Shaw, B. H. Hahn, W. B. Williams, S. Wang, W. Ding, H. Li and B. F. Haynes. Characteristics of Env evolution underlying the development of V3 glycan bNAbs in SHIV-BG505 infected Rhesus Macaques.. Presented at *CHAVI-ID annual retreat*, Los Alamos, New Mexico, United States, 2021-10-11 - 2021-10-14. (LA-UR-21-30008)

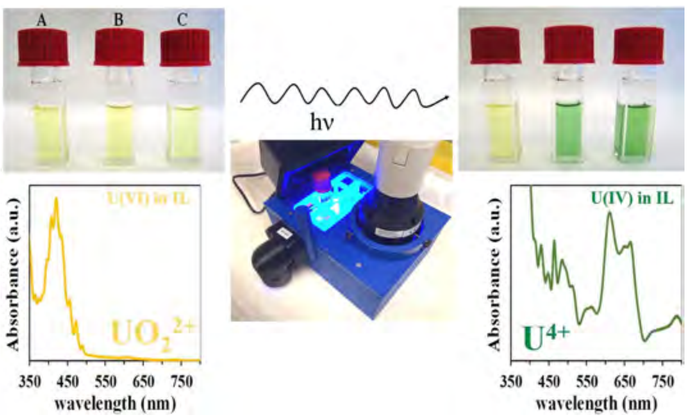
Posters

Goldberg, E. E. Viral Modeling. . (LA-UR-20-26632)

**Peer-reviewed*

Photochemistry of Actinides in Ionic Liquids for Advanced Separations

Janelle Droessler
20200561ECR



The ability of some ionic liquids to promote oxidation state changes with judicious application of the energy of the light source may have applications for advanced actinide separations concepts. For example, two of the three ionic liquids (ILs) have undergone photoreduction of uranyl (UO22+), to uranium oxide (U(IV)). Ultra-violet visible spectroscopy confirms the photoreduction after the IL samples were exposed to a 425 nm light source (glowing photoredox box pictured in center). The ability to photoreduce uranyl in certain ILs appears efficient and may afford alternative means of manipulating oxidation states for actinide separations including transuranics such as plutonium.

Project Description

This project will utilize wavelengths of light to manipulate actinide oxidation states in ionic liquids (ILs). Identification of accessible oxidation states and their stability in ILs would expand our fundamental understanding of actinides in ILs, with broader implications for advanced actinide separations relevant to special nuclear material (SNM) production and nuclear fuel cycles. Actinide redox chemistry has been the foundation of nuclear fuel cycle separations, production of critical materials, and campaigns relevant to the missions of Department of Energy (DOE) and National Nuclear Security Administration (NNSA). DOE workshops have also included a call for further work related to ILs for nuclear separations technology, yet little has been done. The proposed research is strongly aligned with the Integrated Plutonium Science and Research Strategy. The fundamental science developed in this project could also be employed for advanced actinide separations technologies useful for a variety of other Lab/DOE missions including stockpile stewardship (production/disposition of SNM), energy security (nuclear fuel cycles), and global security (proliferation).

Technical Outcomes

The outcomes of the project show that structure of the ionic liquid significantly impacts photoreduction of the actinide versus other reactions (competition/efficiency). The rate of reaction can also be driven by selection of the light wavelength to overlap with the maximum electronic excitation of the actinide species. Additional data supports hydrogen abstraction as part of the mechanism which likely involves a uranium intermediate and disproportionation.

Publications

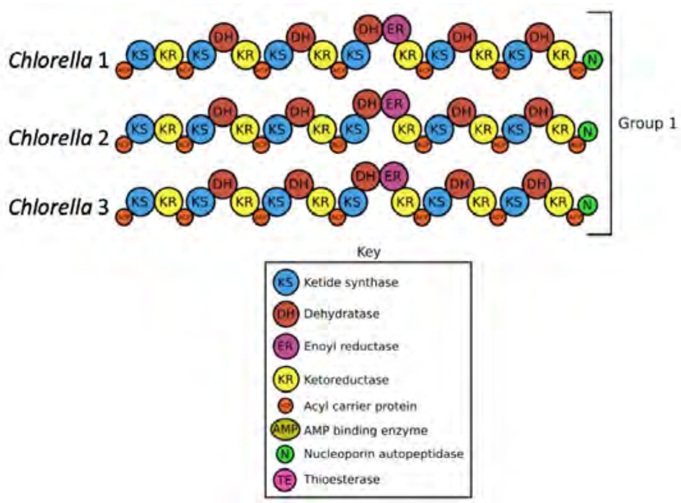
Presentation Slides

Droessler, J. E., K. S. Boland, G. S. Goff, M. C. F. Rier and L. E. Wolfsberg. Photochemistry of Uranyl in Ionic Liquids for Advanced Separations. Presented at *Actinide Separations Conference*, Los Alamos, New Mexico, United States, 2022-05-17 - 2022-05-19. (LA-UR-22-24539)

**Peer-reviewed*

Computational and Experimental Bioprospecting of Algae for Antimicrobial Compounds

Blake Hovde
20200562ECR



We are developing a method for identification and classification clustering algorithm to classify potential antibiotic genes in algae for new antibiotic discovery. This image shows some of the alignments of polyketide synthase gene structures within the three different Chlorella algae.

Project Description

The declining number of new antibiotics reaching the market is extremely concerning, as increasingly resistant bacteria pathogens continue to propagate worldwide. Antimicrobial resistance is designated by the Centers for Disease Control and Prevention (CDC) as one of the “biggest public health challenges in our time” as drug resistant Staphylococcus and Streptococcus infections alone caused 40,000 deaths in the United States in 2017. Algae represent a significantly diverse group of organisms as well as wholly untapped resource for new antibiotic discovery. To identify new algal antimicrobial compounds in order to combat the serious issue of globally increasing antimicrobial resistance, this project will utilize two critical and unique resources that are available at Los Alamos that will allow this research to lead the field of algae bio-prospecting for new antibiotics. These unique resources include our world leading curation of over 130 algal genomes collected to date that we will use to mine these genomes for new antibiotic genes. Additionally, a new Los Alamos microfluidics technology "HiSCI" (High-throughput screening of cell-to-cell interactions) will allow for biological screening of antibiotic compounds from algae obtained from ocean and lake environments.

Technical Outcomes

Algae were confirmed to have a high potential for novel antibiotic compounds. The project generated a large (almost doubling) set of algal genomes for the greater algae research. Predicting algal antibiotic compound function reliably may not yet be wholly feasible using the computation methods developed over the course of this project. Experimental cloning of the top candidate antibiotic gene selections may remedy this lingering question.

Publications

Journal Articles

Biondi, T. C., C. P. Singer Kruse, S. I. Koehler, T. Kwon, W. L. K. M. Eng, Y. A. Kunde, C. D. Gleasner, K. T. You Mak, J. E. W. Polle, B. Hovde, E. R. Hanschen and S. R. Starkenburg. Assembly and analysis of the 100% complete, gapless, phased diploid genome of Scenedesmus obliquus UTEX 3031. Submitted to *Nucleic Acids Research*. (LA-UR-22-31391)

Hovde, B., K. R. Fixen, R. A. Cattolico, C. R. Deodato and E. R. Hanschen. Transcriptional profiling of the haptophyte Chrysochromulina tobinii and its associated phycosphere uncover potential algal-bacterial interactions over a diel photoperiod. Submitted to *Frontiers in Microbiology*. (LA-UR-23-22911)

Kwon, T., B. Hovde and E. R. Hanschen. Addressing the pervasive scarcity of structural annotation in eukaryotic algae. 2023. *Scientific Reports*. **13** (1): 1687. (LA-UR-21-30119 DOI: 10.1038/s41598-023-27881-0)

Kwon, T. and B. Hovde. Genome-guided establishment of encyclopedia of algal natural product. Submitted to *iScience*. (LA-UR-22-20439)

Posters

Hovde, B. and T. Kwon. Introduction to the algal antibiotic resources using in-silico approach. Presented at *Algal Biomass, Biofuels and Bioproducts*, Online Only, New York, United States, 2021-06-14 - 2021-06-16. (LA-UR-21-25507)

Kwon, T., E. R. Hanschen and B. Hovde. Leveraging universal orthologs to recover the algal genome diversity. Presented at *16th Annual Sequencing, Finishing, & Analysis in the Future (SFA\xc2\xb2F) Meeting*, Santa Fe, New Mexico, United States, 2021-09-28 - 2021-09-29. (LA-UR-21-29434)

**Peer-reviewed*

Self-Repairing Subsurface Well Cement to Reduce Climate Change

Nathan Welch
20220549ECR

Leakage of carbon dioxide and carbon dioxide saturated fluids in subsurface wells dissolves well cement used to seal between a steel well casing and a drilled wellbore. This image shows the surface of a cement microfluidic device used to observe the mineral dissolution and precipitation caused by leaking carbon dioxide in well cement along a serpentine flow path and to explore the potential benefit of using lanthanum and cerium as a cement additive to help seal leaking wells.

Project Description

Low-carbon energy technologies rely heavily on critical minerals as identified by the Office of Fossil Energy and Carbon Management, and the domestic production of critical minerals in the United States is essential in providing energy security for the United States. However, the domestic production of critical minerals is cost prohibitive at current market values. The extensive deployment of carbon dioxide (CO2) sequestration is vital in meeting the climate impact goals of the United States, and new well cement technologies can reduce the risk of subsurface leakage of stored carbon dioxide. By developing a new well cement that adds value to low demand rare earth elements, we can support domestic production of critical minerals while reducing risk in subsurface carbon dioxide disposal.

Technical Outcomes

Leakage of carbon dioxide through defects in wellbore cement poses a significant risk to the long-term storage of carbon dioxide in the subsurface as a method to mitigate climate change. This project aimed to enhance the self-sealing properties of cement exposed to CO2 through the addition of the rare earth elements lanthanum and cerium that form stable carbonates. High-pressure microfluidic CO2 flow experiments demonstrated significant promise in abundant precipitation of carbonates compared traditional well cement.

Publications

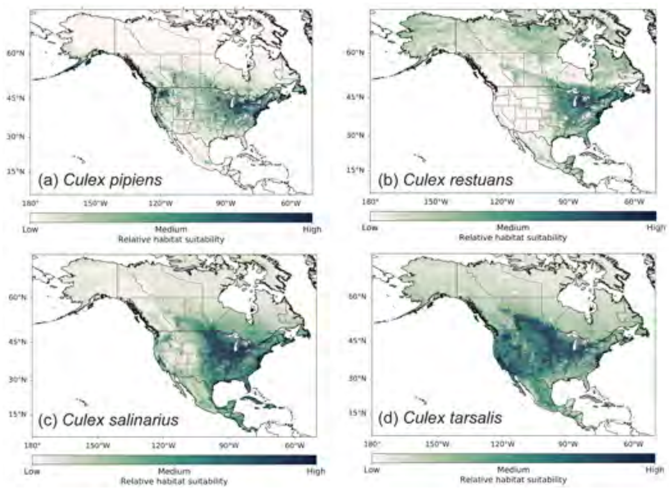
Conference Papers

Welch, N. J., S. K. Peterson, R. J. Harris, S. Abedi, J. W. Carey and H. Boukhalfa. Carbon dioxide disposal well rare earth element enriched cement. Presented at *Conference on Greenhouse Gas Control Technologies (GHGT)*. (Lyon, France, 2022-10-24 - 2022-10-28). (LA-UR-22-29790)

**Peer-reviewed*

Forecasting Valley Fever Disease Risk Using Machine Learning

Morgan Gorris
20200682PRD1



Identifying where important disease vectors live is critical for understanding what communities are at risk of contracting diseases. Culex mosquitoes spread West Nile virus, the largest cause of mosquito-borne illness in humans in the United States. We found that different species are suitable for living throughout different regions.

Project Description

Several recent studies by the National Academy of Sciences and the United States Government have highlighted the implications of climate change on national security and the need for research that integrates complex dynamics to forecast risk. One particular risk driven by climate change is the potential for shifts in the regions affected by infectious diseases. These shifts and the potential for resultant disease outbreaks would pose a threat to national security by affecting human health. This research will strengthen our understanding of the relationships between climate and infectious diseases in order to create disease support tools, such as disease forecasts and projections in response to climate change. Tools and methods for accurate disease forecasting are of interest to numerous United States stakeholders such as the Department of Energy (DOE), Department of Defense (DOD), Department of Homeland Security (DHS), Department of Health and Human Services (HHS), and the United States Department of Agriculture (USDA), and were recently prioritized by the National Biodefense Strategy (2018).

Publications

Journal Articles

*Shaping the Future of Science: COVID-19 Highlighting the Importance of GeoHealth. 2021. *GeoHealth*. **5** (5): e2021GH000412. (LA-UR-21-21425 DOI: 10.1029/2021GH000412)

*Carey, A., M. E. Gorris, T. Chiller, B. Jackson, W. Beadles and B. J. Webb. Epidemiology, Clinical Features, and Outcomes of Coccidioidomycosis, Utah, 2006–2015. 2021. *Emerging Infectious Diseases*. **27** (9): 2269-2277. (LA-UR-20-21991 DOI: 10.3201/eid2709.210751)

. B. A. W. *. T. S. D. *. R. D. *. S. D. P. *. F. J. M. *. K. K. A. *. D. V. S. Y. *. M. C. A. Gorris, M. E., M. E. Gorris, A. W. Bartlow, S. D. Temple, J. M. Fair, K. A. Kaufeld, S. Y. Del Valle, C. A. Manore, D. Romero-Alvarez and D. P. Shutt. Updated distribution maps of predominant Culex mosquitoes across the Americas. 2021. *Parasites & Vectors*. **14 (1): 547. (LA-UR-21-24460 DOI: 10.1186/s13071-021-05051-3)

*Gorris, M. E., A. W. Bartlow, S. D. Temple, D. Romero-Alvarez, D. P. Shutt, J. M. Fair, K. A. Kaufeld, S. Y. Del Valle and C. A. Manore. Updated distribution maps of predominant Culex mosquitoes across the Americas. 2021. *Parasites & Vectors*. **14** (1): 547. (LA-UR-21-24422 DOI: 10.1186/s13071-021-05051-3)

*Gorris, M. E., C. D. Shelley, S. Y. Del Valle and C. A. Manore. A time-varying vulnerability index for COVID-19 in New Mexico, USA using generalized propensity scores. 2021. *Health Policy OPEN*. **2**: 100052. (LA-UR-20-30424 DOI: 10.1016/j.hpopen.2021.100052)

Gorris, M. E., J. T. Randerson, S. R. Coffield, K. K. Treseder, C. S. Zender, C. Xu and C. A. Manore. Climate controls on the spatial pattern of West Nile virus incidence in the United States. Submitted to *Environmental Health Perspectives*. (LA-UR-22-20129)

Gorris, M. E., M. Caballero Van Dyke, A. Carey, P. S. Hamm, H. L. Mead and J. K. Uehling. A Review of Coccidioides Research, Outstanding Questions in the Field, and Contributions by Women Scientists. Submitted to *Current Clinical Microbiology Reports*. (LA-UR-21-23354)

Hoffman-Hall, A., M. E. Gorris, S. Anenberg, A. Bredder, J. K. Dhaliwal, M. A. Diaz, S. K. Fortner, B. McAdoo, D. Reano, R. Rehr, H. Roop and B. F. Zaitchik. A GeoHealth Call to Action: Moving Beyond Identifying Environmental Injustices to Co-Creating Solutions. 2022. *GeoHealth*. **6** (11): e2022GH000706. (LA-UR-22-28540 DOI: 10.1029/2022GH000706)

Holcomb, K. M., M. A. Johansson, S. Mathis, C. M. Baker, J. E. Staples, M. Fischer, R. J. Nett, C. B. Beard, E. A. Mordecai, M. L. Childs, D. Kirk, M. J. Harris, N. Nova, M. P. Kain, A. C. Keyel, I. Rochlin, M. Marcantonio, E. L. Ray, J. M. Humphreys, L. W. Cohnsteadt, B. D. Hollingsworth, E. M. Reed, A. S. Freedman, M. Hamins-Puertolas, P. Das and M. E. Gorris. Evaluation of an open forecasting challenge to assess skill of West Nile virus neuroinvasive disease prediction. Submitted to *Parasites and Vectors*. (LA-UR-22-26001)

*Keyel, A. C., M. E. Gorris, I. Rochlin, J. A. Uelmen, L. F. Chaves, G. L. Hamer, I. K. Moise, M. Shocket, A. M. Kilpatrick, N. B. Defelice, J. K. Davis, E. Little, P. Irwin, A. J. Tyre, K. H. Smith, C. L. Fredregill, O. E. Timm, K. M. Holcomb, M. C. Wimberly, M. J. Ward, C. M. Barker, C. G. Rhodes and R. L. Smith. A proposed framework for the development and qualitative evaluation of West Nile virus models and their application to local public health decision-making. 2021. *PLOS Neglected Tropical Diseases*. **15** (9): e0009653. (LA-UR-21-22349 DOI: 10.1371/journal.pntd.0009653)

Tong, D. Q., M. E. Gorris, T. E. Gill, K. Ardon-Dryer, J. Wang and L. Ren. Dust Storms, Valley Fever, and Public Awareness. 2022. *GeoHealth*. **6** (8): e2022GH000642. (LA-UR-22-22270 DOI: 10.1029/2022GH000642)

Treseder, K. K., C. J. Alster, L. A. Cat, M. E. Gorris, A. L. Kuhn, K. G. Lovero, F. Hagedorn, J. F. Kerekes, T. A. McHugh and E. F. Solly. Nutrient traits linked to fungal responses to global change. Submitted to *Elementa: Ecology and Earth Systems*. (LA-UR-20-27381)

Books/Chapters

Ebi, K. L., M. H. Hayden, M. E. Gorris, C. Uejio and J. Vanos. Chapter 15: Uncertainty in determining impacts of climate change on human health. (LA-UR-22-28552)

Reports

Germann, T. C., M. Z. Smith, L. R. Dauelsberg, G. Fairchild, T. Turton, M. E. Gorris, C. M. Watson Ross, J. P. Ahrens, D. D. Hemphill, C. A. Manore and S. Y. Del Valle. Using an Agent-Based Model to Assess School Re-openings Under Different COVID-19 Spread Scenarios. Unpublished report. (LA-UR-20-27982)

Presentation Slides

Gorris, M. E. Projecting the risk of environmental infectious diseases in response to climate change. Presented at *US CLIVAR webinar*, Los Alamos, New Mexico, United States, 2021-05-19 - 2021-05-19. (LA-UR-21-24860)

Gorris, M. E. Using climate and environmental data to understand Valley fever disease dynamics. . (LA-UR-21-31356)

Gorris, M. E. Life at LANL as an Earth System Scientist, and the new field of GeoHealth. . (LA-UR-22-25545)

Gorris, M. E. The projected expansion of coccidioidomycosis (Valley fever) endemic regions in response to climate change. Presented at *ZOHU Call: Zoonoses & One Health Update*, Los Alamos, New Mexico, United States, 2022-09-07 - 2022-09-07. (LA-UR-22-29039)

Gorris, M. E. Using climate and environmental data to understand Valley fever disease dynamics. Presented at *Health Officers Association of California*, Los Alamos, New Mexico, United States, 2022-10-14 - 2022-10-14. (LA-UR-22-30977)

Gorris, M. E., J. Neumann, P. Kinney, M. Sheahan and M. Sarofim. Economic valuation of Valley fever (coccidioidomycosis) in response to climate change. Presented at *American Geophysical Union Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31689)

Gorris, M. E., K. Treseder, C. Zender and J. Randerson. The expansion of Valley fever endemic regions in response to climate change. Presented at *NM Dust Symposium*, Los Alamos, New Mexico, United States, 2021-10-27 - 2021-10-27. (LA-UR-21-30328)

Gorris, M. E., P. L. Kinney, J. E. Neumann and M. C. Sarofim. Using precipitation to forecast coccidioidomycosis incidence in the San Joaquin Valley of California. Presented at *Coccidioidomycosis Study Group Annual Meeting*, Los Alamos, New Mexico, United States, 2021-04-16 - 2021-04-17. (LA-UR-21-23582)

Gorris, M. E., T. C. Germann, L. R. Dauelsberg, C. M. Watson Ross, G. Fairchild, M. Z. Smith, J. P. Ahrens, D. D. Hemphill, C. A. Manore and S. Y. Del Valle. Using an agent-based model to assess school reopening scenarios in response to COVID-19. . (LA-UR-21-22491)

Manore, C. A. COVID-19 Modeling for Pandemic Response. Presented at *Public Health Data to Action*, Santa Fe, New Mexico, United States, 2020-11-19 - 2020-11-19. (LA-UR-20-29491)

Shelley, C. D. and M. E. Gorris. Designing a dynamic vulnerability index to COVID-19 for New Mexico, USA. . (LA-UR-20-26076)

Other

Gorris, M. E., A. W. Bartlow, S. D. Temple, D. A. Romero-Alvarez, D. A. Shutt, J. M. Fair, K. A. Kaufeld, S. Y. Del Valle and C. A. Manore. netCDF files of Culex habitat suitability values. Dataset. (LA-UR-21-24576)

**Peer-reviewed*

Predicting Pan-arctic Permafrost Collapse with Next-generation Data Analytics and Models

Charles Abolt
20200771PRD4

Survey areas in the present analysis. Red dots indicate survey areas where the area of thermokarst pools has abruptly increased in the past thirteen years. These survey areas are disproportionately located in uplands containing topographically convex features.

Project Description

The proposed work will provide fundamental understanding of how Arctic landscapes will thaw in response to climate change, and its impact on ground stability. This new knowledge will be available to decision makers as they plan land and coastal infrastructure development under future climate conditions in vast Arctic areas that are of strategic importance for power interactions, energy development, new global transportation routes, and commercial opportunities.

Publications

Journal Articles

Abolt, C. J., A. L. Atchley, D. R. Harp, A. K. Liljedahl, M. T. Jorgenson, C. Witharana, W. R. Bolton, J. P. Schwenk, T. Rettelbach, G. Grosse, J. Boike, I. Nitze, C. Rumpca, C. J. (. Wilson and K. E. Bennett. Topography drives variability in circumpolar permafrost thaw pond expansion. Submitted to *Nature Climate Change*. (LA-UR-22-24831)

Abolt, C. J., A. L. Atchley, D. R. Harp, A. K. Liljedahl, M. T. Jorgenson, C. Witharana, W. R. Bolton, J. Schwenk, T. Rettelbach, G. Grosse, J. Boike, I. Nitze, C. T. Rumpca, C. J. (. Wilson and K. E. Bennett. Topography drives variability in circumpolar permafrost thaw pond expansion. Submitted to *Nature*. (LA-UR-21-32264)

Abolt, C. J., J. Nitzbon, M. Langer and A. L. Atchley. Reducing uncertainty in simulations of enhanced permafrost thaw beneath thermokarst pools. Submitted to *Cryosphere*. (LA-UR-22-30471)

Presentation Slides

Abolt, C. J., A. L. Atchley, D. R. Harp, A. K. Liljedahl, M. T. Jorgenson, C. Witharana, W. R. Bolton, J. P. Schwenk, T. Rettelbach, G. Grosse, J. Boike, I. Nitze, C. Rumpca, C. J. (. Wilson and K. E. Bennett. Topography drives variability in circumpolar permafrost thaw pond expansion. Presented at *2022 DOE ESS PI Meeting*, Bethesda, Maryland, United States, 2022-05-24 - 2022-05-26. (LA-UR-22-24830)

Abolt, C. J., A. L. Atchley, D. R. Harp, A. K. Liljedahl, M. T. Jorgenson, C. Witharana, W. R. Bolton, T. Rettelbach, J. P. Schwenk, C. T. Rumpca and C. J. (. Wilson. Circumpolar observations of thermokarst pool expansion from high-resolution satellite imagery. Presented at *Regional Conference on Permafrost (online)*, Boulder, Colorado, United States, 2021-10-24 - 2021-10-29. (LA-UR-22-20761)

Abolt, C. J., A. L. Atchley, D. R. Harp, A. Liljedahl, T. Jorgenson, C. Witharana, B. Bolton, T. Rettelbach, C. T. Rumpca and C. J. (. Wilson. Circumpolar observations of thermokarst pool expansion in high-resolution satellite imagery. Presented at *Permafrost Discovery Gateway online seminar*, Los Alamos, New Mexico, United States, 2021-07-22 - 2021-07-22. (LA-UR-22-20759)

Abolt, C. J., A. L. Atchley, S. L. Painter and K. E. Bennett. Integrated modeling and observations of ground deformation in polygonal tundra, Alaska North Slope. Presented at *NGEE Arctic All Hands Online Meeting 2022*, Los Alamos, New Mexico, United States, 2022-02-15 - 2022-02-17. (LA-UR-22-21108)

Abolt, C. J., J. Nitzbon, M. Langer and A. L. Atchley. Reducing uncertainty in simulations of thaw in ice-rich permafrost. Presented at *American Geophysical Union (AGU) Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32286)

Abolt, C., A. Atchley, D. Harp, A. Liljedahl, T. Jorgenson, C. Witharana, C. T. Rumpca and C. J. Wilson. Circumpolar observations of ice wedge melting and thermokarst pool expansion. . (LA-UR-21-21713)

Abolt, C., A. Atchley, M. Young, D. Harp, C. Rumpca and C. Wilson. Integrated modeling and observations of ice wedge degradation and thermokarst pool expansion. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29443)

Abolt, C., A. L. Atchley, D. R. Harp, C. T. Rumpca and C. J. Wilson. Pan-Arctic observations of ice wedge melting and thermokarst pool expansion. Presented at *NGEE Arctic All Hands 2021 Meeting*, Oak Ridge, Tennessee, United States, 2021-01-26 - 2021-01-28. (LA-UR-21-20932)

Posters

Abolt, C., A. Atchley, D. Harp, A. Liljedahl, T. Jorgenson, C. Witharana, C. Rumpca and C. Wilson. Topography drives variability in circumpolar ground ice vulnerability. Presented at *Arizona Days (online)*, Los Alamos, New Mexico, United States, 2021-05-17 - 2021-05-17. (LA-UR-21-24720)

Other

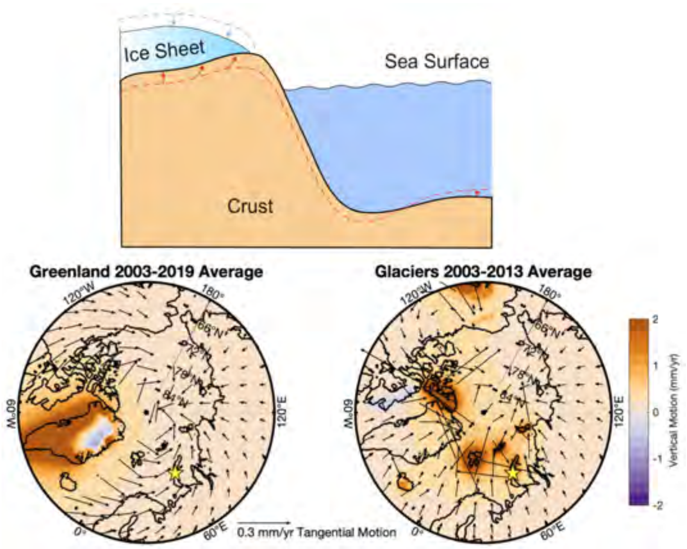
Abolt, C. J., A. L. Atchley, D. R. Harp and C. T. Rumpca. Maps of thermokarst pool expansion at 27 Arctic survey areas. Dataset. (LA-UR-21-32379)

Rumpca, C. T., C. J. Abolt, A. L. Atchley and D. R. Harp. Tool and training data for cloud detection in WorldView satellite imagery. Dataset. (LA-UR-21-32378)

**Peer-reviewed*

Climate Change-induced Seismicity? Quantifying the Impact of Ice and Ocean Loading on Crustal Stress and Seismicity in the Russian Arctic

Matthew Hoffman
20210952PRD3



Changing ice and water loads on the Earth's surface result in viscoelastic deformation of the Earth's crust (top). The figures show modeled crustal motion induced by mass loss of the Greenland Ice Sheet (left) and a global inventory of mountain glaciers (right). Vertical motion is shown in color and tangential motion is represented as arrow vectors. The associated modification to the crust's stress field can be calculated from these deformation fields, and has the potential to alter earthquake activity. These stress changes will be compared to existing earthquake catalogs, focusing on the island Novaya Zemlya (yellow star). Credit: Sophie Coulson.

Project Description

Recent studies have focused on assessing melting of glaciers and the associated sea-level rise caused by climate change. However, this redistribution of water across Earth's surface also causes the solid Earth to deform in response to the local reduction or increase in mass sitting on the Earth's crust. This project will assess whether this crustal bending, due to climate-change-induced glacial melting over the last several decades, has been significant enough to alter earthquake activity. We focus on the Russian Arctic, where determining the cause of earthquakes is paramount for national security, as natural seismicity in this region can mask seismicity generated by nuclear testing. Bending of the crust in this region is affected by melting of the Arctic glaciers it is surrounded by, as well as significant melting of the Greenland Ice Sheet. Assuming a correlation is found, we will use predictions of future climate change to project future earthquake patterns and identify other regions sensitive to these processes worldwide. This research has the potential to identify increasing earthquake hazard as an unidentified impact of climate change. The project supports Department of Energy's mission by linking existing ocean and ice sheet modeling capabilities to climate impacts relevant to national security.

Publications

Journal Articles

Borreggine, M., K. Latychev, S. L. Coulson, E. M. Powell, J. X. Mitrovica, G. A. Milne and R. B. Alley. Sea-Level Rise in Southwest Greenland as a Driver of Viking Out-Migration. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-22-29976)

Coulson, S. L., M. Lubeck, J. X. Mitrovica, E. Powell, J. L. Davis and M. J. Hoggard. The Global Fingerprint of Modern Ice-Mass Loss on 3-D Crustal Motion. 2021. *Geophysical Research Letters*. **48** (16): e2021GL095477. (LA-UR-21-27647 DOI: 10.1029/2021GL095477)

*Coulson, S., S. Dangendorf, J. X. Mitrovica, M. E. Tamisiea, L. Pan and D. T. Sandwell. A detection of the sea level fingerprint of Greenland Ice Sheet melt. 2022. *Science*. **377** (6614): 1550-1554. (LA-UR-22-20175 DOI: 10.1126/science.abo0926)

*Onac, B. P., J. X. Mitrovica, J. Gines, Y. Asmerom, V. J. Polyak, P. Tuccimei, E. L. Ashe, J. J. Fornos, M. J. Hoggard, S. Coulson, A. Gines, M. Soligo and I. M. Villa. Exceptionally stable preindustrial sea level inferred from the western Mediterranean Sea. 2022. *Science Advances*. **8** (26): eabm6185. (LA-UR-21-29168 DOI: 10.1126/sciadv.abm6185)

Richards, F., S. L. Coulson, M. Hoggard, J. Austermann, B. Dyer and J. X. Mitrovica. Correcting for dynamic topography reconciles estimates of Mid-Pliocene sea level around Australia. Submitted to *Nature*. (LA-UR-22-31677)

Presentation Slides

Coulson, S. L. Predicting and Observing Patterns of Modern Sea Level Change and Crustal Deformation. . (LA-UR-22-30867)

Coulson, S. L., M. Lubeck, J. X. Mitrovica, E. Powell, J. Davis and M. Hoggard. The Global Fingerprint of Modern Ice-Mass Loss on 3-D Crustal Motion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31982)

Posters

Coulson, S. L., S. Dangendorf, J. X. Mitrovica, M. E. Tamisiea, L. Pan, D. T. Sandwell and N. Hendricks. A Detection of the Sea Level Fingerprint of Greenland Ice Sheet Melt. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32648)

Coulson, S. L., S. Dangendorf, J. X. Mitrovica, N. Hendricks, M. E. Tamisiea, L. Pan, D. T. Sandwell, K. Han and M. J. Hoffman. Utilization of High-Resolution Ice Mass Balance Datasets for Predicting and Observing Patterns of Sea Level Change. Presented at *Twenty-Ninth Annual WAIS Workshop*, Estes Park, Colorado, United States, 2022-09-26 - 2022-09-29. (LA-UR-22-29936)

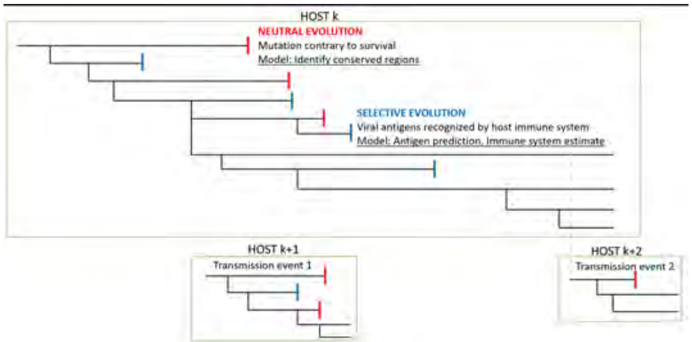
Other

Coulson, S. L., J. M. Patchett and L. Palmstrom. Animation for A Detection of the Sea Level Fingerprint of Greenland Ice Sheet Melt. Audio/Visual. (LA-UR-22-30055)

**Peer-reviewed*

Within and Between Host Scale Integration to Model HIV Transmission

Thomas Leitner
20210959PRD3



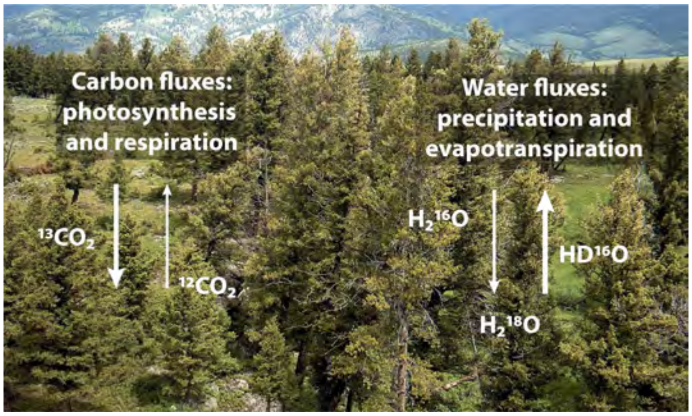
Phylogenetic trees showing evolution of HIV in 3 epidemiologically linked hosts. The project will develop an agent-based, data-driven model of HIV evolution integrating within and between host scales. Lineages can die neutrally (blue) if a mutation contrary to viral survival occurs, modeled by identifying conserved regions. Lineages can also die selectively (red) if viral antigens are recognized by the host immune system, modeled through antigen prediction and immune status estimates. The resulting sequence diversity within a host determines the possible HIV sequences that can seed an infection at each transmission event.

Project Description

We will develop a comprehensive simulation tool that takes within-host Human Immunodeficiency Virus (HIV) genetic variability into account on a detailed level to evaluate how HIV spreads among persons. An enhanced quantitative understanding of HIV transmission can help identify public health policies to reach the objectives set up by Joint United Nations Programme on HIV/Acquired Immunodeficiency Syndrome (UNAIDS) (reaching the 90-90-90 goal), and the 2019 United States Presidential goal of "Ending the HIV epidemic". Thus, this projects addresses Department of Energy/Los Alamos National Laboratory mission objectives in biosecurity and public health.

Using NEON Stable Isotope Data to Improve Ecosystem Simulation in Earth System Models

Katrina Bennett
20210961PRD3



Exchange of water and carbon dioxide between the land and the atmosphere is determined in part by ecosystem structure and function. Naturally occurring stable isotope tracers in atmospheric water vapor and carbon dioxide provide process-level tracers of ecosystem photosynthesis, respiration, and evapotranspiration. The National Ecological Observatory Network represents the first continental-scale observation network of consistently collected water and carbon isotope ratio data associated with flux towers and presents an opportunity to improve representation and validation of ecosystems and their interaction with the atmosphere in earth system models.

Project Description

Ecosystem response to increasing atmospheric temperatures and altered precipitation patterns is complex and poses several challenges to national security from projecting water resource availability to understanding wildland fire risk. Recent severe droughts in the western United States have led to widespread forest mortality events. Land surface models have been developed to represent the complexity of ecosystems and their interaction with the atmosphere, but forest mortality events remain challenging to predict. Subtle geochemical variations in atmospheric water and carbon dioxide arise from a range of climatic and ecosystem processes. These chemical variations provide a ‘fingerprint’ of environmental change that can be used to validate and improve numerical model representation of ecosystem processes, thereby improving our ability to understand ecosystem response to past and future environmental change.

Publications

Journal Articles

*Finkenbiner, C. E., B. Li, L. Spencer, Z. Butler, M. Haagsma, R. P. Fiorella, S. T. Allen, W. Anderegg, C. J. Still, D. Noone, G. J. Bowen and S. P. Good. The NEON Daily Isotopic Composition of Environmental Exchanges Dataset. 2022. *Scientific Data*. **9** (1): 353. (LA-UR-22-23395 DOI: 10.1038/s41597-022-01412-4)

Fiorella, R. P., S. A. Kannenberg, W. R. L. Anderegg, R. K. Monson and J. R. Ehleringer. Heterogeneous isotope effects decouple conifer leaf and branch sugar \xce\xb418O and \xce\xb413C. 2022. *Oecologia*. **198** (2): 357-370. (LA-UR-21-31455 DOI: 10.1007/s00442-022-05121-y)

Hawkins, L. R., M. Bassouni, W. R. L. Anderegg, M. D. Venturas, S. P. Good, H. J. Kwon, C. V. Hanson, R. P. Fiorella, G. J. Bowen and C. J. Still. Comparing Model Representations of Physiological Limits on Transpiration at a Semi-arid Ponderosa Pine Site. 2022. *Journal of Advances in Modeling Earth Systems*. e2021MS002927. (LA-UR-22-26624 DOI: 10.1029/2021MS002927)

Henze, D., D. Noone, S. de Szoeke, G. de Boer, R. P. Fiorella, A. Bailey and P. Blossey. Vertical structure of turbulence and fluxes across cloud mesoscale organizations from the WP-3D Orion aircraft during ATOMIC. Submitted to *Earth and Space Science Open Archive*. (LA-UR-22-31385)

Li, B., S. P. Good, C. E. Finkenbiner, R. P. Fiorella, G. J. Bowen, D. C. Noone, C. J. Still and W. R. L. Anderegg. Stable isotopes contain substantial additive information about carbon and water cycles. Submitted to *Nature Geoscience*. (LA-UR-22-28881)

Presentation Slides

Fiorella, R. P. Using NEON Stable Isotope Data to Improve Ecosystem Simulation in Earth System Models. Presented at *NGEE Arctic All-Hands Meeting (virtual)*, virtual, New Mexico, United States, 2022-02-15 - 2022-02-17. (LA-UR-22-21233)

Fiorella, R. P. Using NEON stable isotope data to understand ecosystem processes and improve Earth system models. . (LA-UR-22-25332)

Fiorella, R. P. Should the NEON ATM ISO TWG recommend changes to peak integration?. . (LA-UR-22-27571)

Fiorella, R. P., K. E. Bennett, C. Xu, B. D. Newman and L. Van Roekel. Ecosystem parameter estimation and model validation using NEON stable isotope ratios. Presented at *NGEE-Arctic All Hands Meeting*, Chattanooga, Tennessee, United States, 2022-10-19 - 2022-10-21. (LA-UR-22-30880)

Hawkins, L. R., S. P. Good, J. C. Fickle, W. R. L. Anderegg, C. M. Jarecke, R. P. Fiorella, D. C. Noone, G. J. Bowen, J. S. Selker and C. J. Still. The importance of soil hydraulic functions in regulating ecosystem drought stress responses in land process models. Presented at *Frontiers in Hydrology Meeting*, San Juan, Puerto Rico, United States, 2022-06-19 - 2022-06-24. (LA-UR-22-25684)

Other

Fiorella, R. P. Calibrated water vapor and carbon dioxide isotope ratios from NEON flux towers. Dataset. (LA-UR-22-22636)

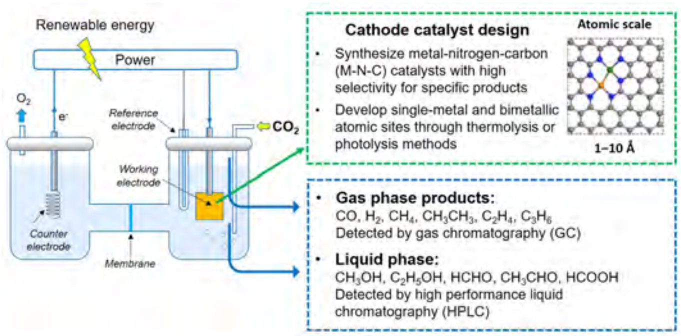
Fiorella, R. P. Gross primary productivity and ecosystem metric estimates derived from NEON flux towers. Dataset. (LA-UR-22-23394)

Fiorella, R. P., S. A. Kannenberg, W. R. L. Anderegg, R. K. Monson and J. R. Ehleringer. Carbon and oxygen isotope ratios of ponderosa pine, Big Cottonwood Canyon, Utah, USA. Dataset. (LA-UR-22-20286)

**Peer-reviewed*

Highly Efficient Electrocatalysts for CO2 Conversion to Value-Added Products

Piotr Zelenay
20210963PRD4



Researchers at Los Alamos National Laboratory focus on the development of selective, high-performance catalysts for electrochemical conversion of CO2 to value-added products such as methanol, ethanol, and ethylene in a hydrogen (H)-type cell (shown), and on the identification and quantification of reaction products by advanced characterization methods, including gas chromatography and high performance liquid chromatography.

Project Description

This project directly addresses the important national security challenge on climate impacts and energy security through eletrochemical carbon dioxide (CO2) conversion to value-added fuels and chemical feedstocks using electricity from renewable sources. The challenge of this technology comes from the competing hydrogen evolution reaction, or water reduction. The key to solving this problem relies on precisely engineering the materials properties for selective reduction of CO2 molecules towards desired product. This project will focus on the development of efficient electrocatalysts to activate the CO2, speed chemical reactions, and selectively generate desired products including carboxylic acids, hydrocarbons, carbon monixide/syngas (Synthesis Gas), and alcohols. Successful demonstration of electrochemical conversion technology will result in a meaningful research portfolio, subsequently drawing industrial interest. Such an interest will ultimately lead to either collaborative or work-for-others projects funded by the private sector.

Publications

Presentation Slides

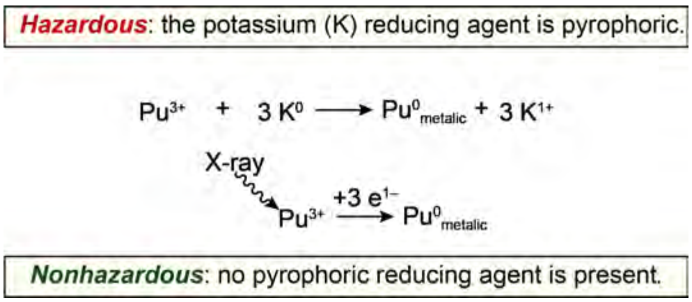
He, Y., J. C. Weiss, J. D. Jernigen and P. Zelenay. Me-N-C Electrocatalysts for Electrochemical CO2 Reduction to High-Value Products. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30428)

He, Y., J. C. Weiss and P. Zelenay. Effect of Nanostructure and Surface Chemistry on Activity and Selectivity of Cu-Based Electrocatalysts for Carbon Dioxide Reduction. Presented at *Electrochemical Society (ECS) Spring Meeting*, Vancouver, Canada, 2022-05-29 - 2022-06-02. (LA-UR-22-24965)

**Peer-reviewed*

X-Ray Mediated Photochemistry of Plutonium

Stosh Kozimor
20210964PRD4



This project will develop use of X-rays as photo-initiators for plutonium (Pu) redox chemistry. Although a representative reduction is shown, oxidation chemistry will be explored as well.

Project Description

The goal of this project is to provide alternative valence adjustment agents used during processing of plutonium containing waste. If successful, this project will lay the ground work for removing harsh chemical agents from waste streams and reduce hazards of effluent form plutonium processing efforts.

Publications

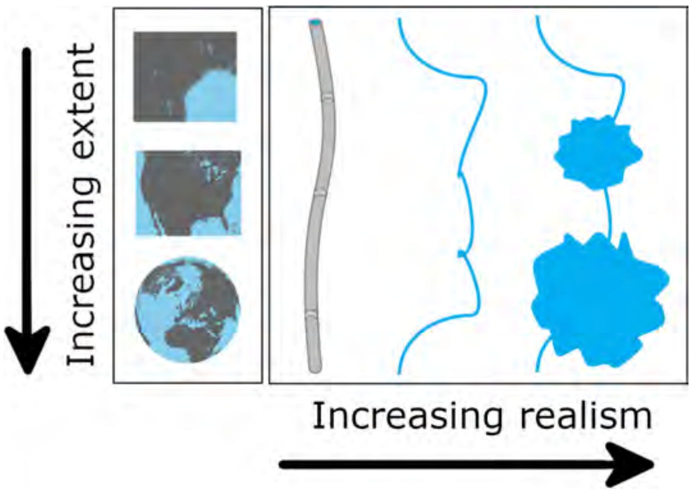
Journal Articles

Rice, N. T., E. Danielou Dalodiere, S. L. Adelman, Z. R. Jones, S. A. Kozimor, V. Mocko, H. D. Root and B. Stein. OXIDIZING AMERICIUM(III) WITH SODIUM BISMUTHATE IN ACIDIC AQUEOUS SOLUTIONS. Submitted to *Inorganic Chemistry*. (LA-UR-22-21284)

**Peer-reviewed*

The Role of Lakes in Global Phosphorus Cycling and Sensitivity to Climate Change

Jonathan Schwenk
20220697PRD1



Emerging evidence suggests that lakes play a critical role in regulating excess nutrient loading in freshwater systems. Such inputs are critical to food and water security as they are responsible for fish kills, drinking water contamination, and toxic algal blooms that are hazardous to human health. Los Alamos National Laboratory is building global models of nutrient flux through lake-river networks that integrate modeling, simulation, and sensing sciences to improve predictability of this important yet understudied ecosystem type. This work moves the state-of-the-science beyond passive transport through "pipes" to actively integrate landscape features such as lakes. [Image credit: Los Alamos National Laboratory]

Project Description

The proposed work will increase the Department of Energy's (DOE) capabilities in the areas of food and water security assessment because excess nutrient loading (particularly from phosphorus) is directly tied to increased incidence of fish kills, contamination of drinking water, and toxic algal blooms which are hazardous to human health. In addition, more detailed knowledge of lake phosphorus retention as a result of the proposed work has the potential to inform better nutrient management strategies and to provide the information necessary to forecast specific lake systems where retention capacity is likely to be overwhelmed by rapid climate change effects.

Publications

Journal Articles

Stachelek, J. Quantifying uncertainty in Pareto estimates of global lake area. Submitted to *Limnology and Oceanography: Methods*. (LA-UR-21-30122)

Swedberg, K., K. J. Boyle, J. Stachelek, N. K. Ward, W. Weng and K. M. Coburn. Examining Implicit Price Variation for Lake Water Quality. Submitted to *Water Economics and Policy*. (LA-UR-22-28690)

Wander, H., R. Chapina, A. Bah, M. J. Farrugia, R. Ghosh, M. Korver, S. La Fuente, E. Massa, E. Munthali, J. Robinson, J. Stachelek, A. Khandelwal, P. C. Hanson and K. C. Weathers. Using knowledge-guided machine learning to assess patterns of areal change in waterbodies across the contiguous US. Submitted to *Environmental Science & Technology*. (LA-UR-23-21976)

Weng, W., K. M. Coburn, A. R. Kemanian, K. J. Boyle, S. Yuning, J. Stachelek and C. White. Quantifying Co-Benefits of Water Quality Policies: An Integrated Assessment Model of Land and Nitrogen Management. Submitted to *American Journal of Agricultural Economics*. (LA-UR-22-28689)

Reports

Stachelek, J., J. Schwenk, P. Regier and N. D. Ward. Uncertainty in global time-resolved methane emissions from aquatic waterbodies. Unpublished report. (LA-UR-23-22015)

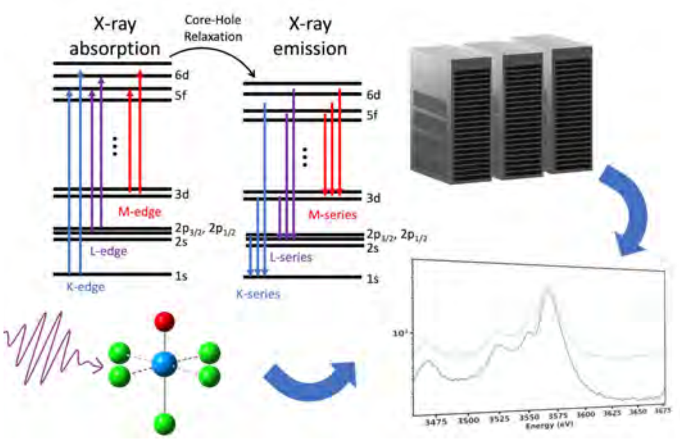
Posters

Stachelek, J. and J. Schwenk. Identifying false positive lakes in surface water detection datasets. Presented at *HydroML Symposium*, State College, Pennsylvania, United States, 2022-05-18 - 2022-05-18. (LA-UR-22-23710)

**Peer-reviewed*

Emission Spectroscopy for Unraveling Actinide Signatures: A Novel Theoretical Approach

Ping Yang
20220701PRD1



Accurate theoretical prediction of X-ray emission spectra (XES) of heavy elements remains challenging due to relaxation in the excited state. The development of new computational methods will enable researchers to distinguish between similar spectra and provide a new tool for forensics of nuclear materials.

Project Description

Nuclear forensics is a key component of the Deparment of Energy (DOE)/National Nuclear Security Administration's (NNSA) mission of stockpile stewardship and deterrence. X-ray emission spectroscopy (XES) is a sensitive technique that can distinguish between similar chemical compounds. However, current computational methods are not accurate enough to predict the small energy shifts in heavy element (for example, uranium or plutonium) XES. This project seeks to combine several developments in computational chemistry to solve this challenge and quantitatively predict the spectroscopic signatures for heavy element XES. Accurate prediction of these small chemical changes will allow DOE/NNSA to identify various nuclear materials with confidence. Computational results for a series of uranium, neptunium, plutonium, and americium will be compared with experimental data to validate the approach.

Publications

Journal Articles

Hartline, D. R., S. T. L\xc3\xb6ffler, D. Fehn, J. M. Kasper, F. W. Heinemann, P. Yang, E. R. Batista and K. Meyer. Utilization of an Endoperoxide as a Potential Surrogate for Molecular Dioxygen in Organouranium Complexes. Submitted to *Journal of the American Chemical Society*. (LA-UR-22-32088)

*Kasper, J. M., X. Li, S. A. Kozimor, E. R. Batista and P. Yang. Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes. 2022. *Journal of Chemical Theory and Computation*. **18** (4): 2171-2179. (LA-UR-21-25945 DOI: 10.1021/acs.jctc.1c00851)

Liao, C. H., J. M. Kasper, A. J. Jenkins, P. Yang, E. R. Batista, M. J. Frisch and X. Li. State Interaction Linear Response Time-Dependent Density Functional Theory with Perturbative Spin-Orbit Coupling: Benchmark and Perspectives. 2023. *JACS Au*. **3** (2): 358-367. (LA-UR-22-32354 DOI: 10.1021/jacsau.2c00659)

Presentation Slides

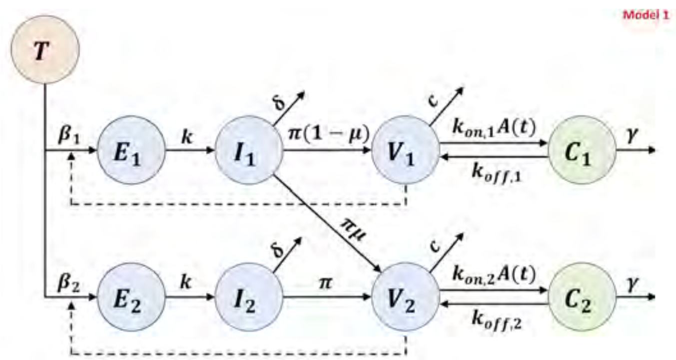
Kasper, J. M., S. M. Greer, J. A. Bradley, D. L. Clark, J. M. Keith, B. E. Klamm, X. Li, S. A. Kozimor, S. G. Minasian, V. Mocko, G. T. Seidler, D. K. Shuh, B. Stein, G. Tian, A. Tondreau, T. Tylisczcak, E. R. Batista and P. Yang. Determining trends in actinyl bonding and the inverse trans-influence using oxygen K-edge X-ray spectroscopy. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-22024)

Kasper, J. M., X. Li, S. A. Kozimor, E. R. Batista and P. Yang. Which Relativistic Approximations are Necessary and When For Modeling the X-ray Spectroscopy of Actinides?. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28778)

**Peer-reviewed*

Mathematical Modeling for SARS-CoV-2 Infection and Resistance Dynamics

Ruian Ke
20220791PRD2



Drug resistance is a result of complex interactions between viral infection and drug action. LANL is using mathematical models (an example schematic is shown above) to understand SARS-CoV-2 resistance to therapies using monoclonal antibodies.

Project Description

The Coronavirus (COVID-19) pandemic has led to an estimate of over five million deaths so far. To mitigate the loss of lives, emergency authorization was given to monoclonal antibody therapies, specifically bamlanivimab (BAM), for treatments of Severre Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) patients with high risk of progressing to severe disease. Preliminary data showed the occurrence of viral rebounds in some patients treated with BAM, leading to more severe diseases. This raises an urgent concern for the development of drug resistance that could compromise the efficacy of this treatment option for severely infected individuals. Drug resistance likely arises from complex nonlinear interactions between virus, host-cells and host immune responses. In this project, we will build a mechanistically descriptive models of the immune system and the within-host infections of SARS-CoV-2 and iterate them using several sets of experimental/clinical data. We will formulate models to capture the mode of action of BAM while considering the presence of natural antibodies to better understand the determinants of its efficacy. The project will lead to identification of effective strategies to manage and mitigate the risk of SARS-CoV-2 drug resistance in clinics and thus is directly relevant to the Global Security Mission within the Department of Energy (DOE)/National Nuclear Security Administration (NNSA).

Publications

Journal Articles

*Meade, W., A. Weber, P. Tin, E. Hampston, L. F. Resa, J. Nagy and Y. Kuang. High Accuracy Indicators of Androgen Suppression Therapy Failure for Prostate Cancer-A Modeling Study. 2022. *Cancers*. **14** (16): 4033. (LA-UR-22-25895 DOI: 10.3390/cancers14164033)

Pell, B., S. Brozak, T. T. Phan, F. Wu and Y. Kuang. A wastewater-based harmless delay differential equation model to understand the emergence of SARS-CoV-2 variants. Submitted to *Journal of Mathematical Biology*. (LA-UR-22-29256)

Perelson, A. S. and T. T. Phan. Viral dynamic models provide a simple explanation for the rebound of SARS-CoV-2 after Paxlovid treatment. Submitted to *PNAS*. (LA-UR-22-29505)

Phan, T. T., A. Weber, A. H. Bryce and Y. Kuang. The prognostic value of androgen to PSA ratio in predictive modeling of prostate cancer. Submitted to *Prostate cancer and prostatic diseases*. (LA-UR-22-30787)

Phan, T. T., J. Bennett and T. Patten. Practical understanding of cancer model identifiability in clinical applications. Submitted to *Life*. (LA-UR-23-20938)

Phan, T. T., S. Brozak, B. Pell, R. M. Ribeiro, R. Ke, A. S. Perelson, Y. Kuang and F. Wu. Making Waves: Integrating wastewater-surveillance data with mathematical modeling to track and predict the trajectory of an outbreak.. Submitted to *Water Research*. (LA-UR-23-20939)

Phan, T. T., S. Brozak, B. Pell, Y. Kuang and F. Wu. A simple SEIR-V model to estimate infectious COVID-19 cases and predict viral transmission using wastewater-based surveillance data. Submitted to *Water Research*. (LA-UR-22-26770)

Phan, T. T. and Y. Kuang. Rich dynamics of a general producer-grazer interaction model under shared multiple resource limitations. Submitted to *Applied Sciences*. (LA-UR-23-20475)

Presentation Slides

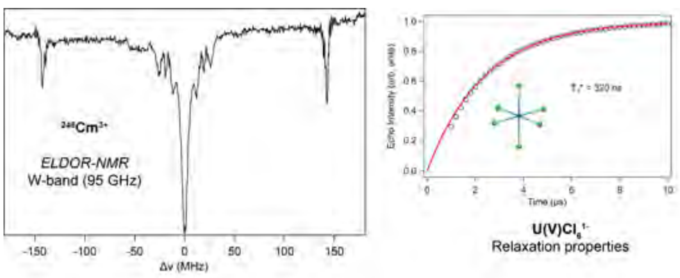
Phan, T. T. Modeling viral resistance to monoclonal antibody monotherapy for SARS-CoV-2. Presented at *Arizona-Los Alamos Days 2022*, Los Alamos, New Mexico, United States, 2022-08-15 - 2022-08-16. (LA-UR-22-28501)

Phan, T. T., C. Zitzmann, A. S. Perelson, R. M. Ribeiro and R. Ke. Modeling viral resistance to monoclonal antibody monotherapy for SARS-CoV-2. Presented at *Biology and medicine through mathematics conference*, Richmond, Virginia, United States, 2022-05-18 - 2022-05-20. (LA-UR-22-23931)

**Peer-reviewed*

Investigating Actinide-Based Molecular Magnetism with Electron Paramagnetic Resonance

Benjamin Stein
20180759PRD4



Electron magnetic resonance techniques are one of the most sensitive ways to understand the details of the magnetic properties of atoms and molecules. This helps explain concepts as diverse as chemical reactivity and suitability for quantum information purposes. This project has multiple "firsts" to its credit, shown here is (left) the first pulsed EPR of a transuranic element (curium in this case), which shows unique behavior as compared to its lanthanide partner gadolinium. (Right) shows the first high-field pulsed EPR of any actinide (here uranium), as well as its magnetic relaxation behavior which defines its suitability for qubit purposes.

Project Description

Beyond their fundamentally interesting chemistry, actinides are an essential aspect of the nuclear weapons enterprise and nuclear energy. Understanding of the detailed relationship between chemical properties and the atomic structure of actinides is important to challenges as diverse as plutonium aging, actinide separations for reprocessing efforts, and plutonium electrorefining. This project seeks to apply modern, advanced magnetic techniques to both improve the understanding of actinides as a whole, and advance the research needs of the field of molecular magnetism. The latter has impacts on areas such as quantum computing and molecular information storage, both areas with significant recent interest (including in areas of national security).

Technical Outcomes

This project advanced understanding of actinide electronic structure and magnetic properties. The team developed containment strategies and safety procedures for performing transuranic electron paramagnetic resonance (EPR) measurements at the National High Magnetic Field Laboratory (NHMFL). The project team performed the first ever high field EPR measurement on a transuranic coordination complex as well as the first pulsed EPR measurement on transuranic materials. These results allow detailed understanding of subtleties of properties of these transuranic ions.

Publications

Journal Articles

P. Goodwin, C. A., M. J. Giansiracusa, S. M. Greer, H. M. Nicholas, P. Evans, M. Vonci, S. Hill, N. F. Chilton and D. P. Mills. Isolation and electronic structures of derivatized manganocene, ferrocene and cobaltacene anions. Submitted to *Nature Chemistry*. (LA-UR-20-23398)

Klamm, B. E., C. J. Windorff, C. Celis-Barros, M. J. Beltran-Leiva, J. M. Sperling, S. M. Greer, M. Y. Livshits, B. Stein and T. E. Albrecht-Schmitt. Exploring the Oxidation States of Neptunium in Schiff Base Coordination Complexes. Submitted to *Chemical Science*. (LA-UR-20-23692)

Presentation Slides

Greer, S. M. Electron paramagnetic resonance studies of f-element complexes. Presented at *From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25504)

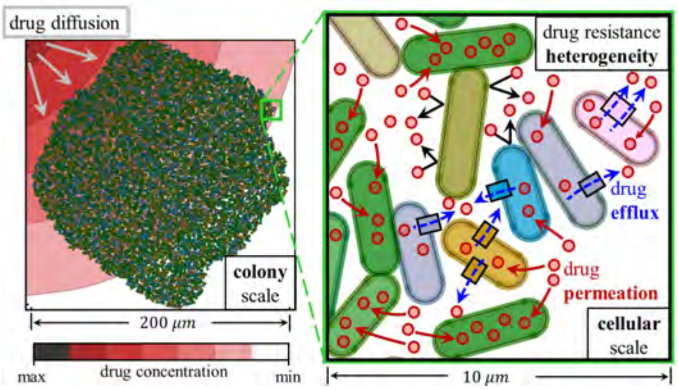
Posters

Greer, S. M., R. Meyer, K. E. Aldrich, J. Marbey, K. Kundu, L. M. Lilley, S. Hill, S. A. Kozimor and B. Stein. Applications of Advanced Electron Paramagnetic Resonance Techniques to Actinide-Based Coordination Complexes. Presented at *Molecular Magnetism in North America*, St Simon Island, Georgia, United States, 2020-02-21 - 2020-02-24. (LA-UR-20-21656)

**Peer-reviewed*

Multiscale Quantitative Description of Drug Resistance Mechanisms in Bacterial Systems

Sandrasegaram Gnanakaran
20190644PRD3



Antibiotic resistance is a growing public health crisis. A crucial challenge is to describe how bacteria pathogens protect, at different levels of resolution, from the drugs that we designed to kill them. LANL has designed, constructed and analyzed a multi-scale mathematical framework able to account for critical mechanisms of resistance and integrate them into a single quantitative model. Quantifying these processes at different functional levels contributes in the design of new and promising protocols at countering antibiotic resistance. [Image credit: Los Alamos National Laboratory]

Project Description

This project builds foundational capability for designing next-generation antibacterial drugs; with a focus on countermeasure development for treating pathogen infection; the understanding gained in this project will have broad applications in biosecurity. At present, we rely on antibiotics for the treatment of bacterial infections encountered in public health and bio-threat scenarios; however, the rapid emergence of antibiotic resistance poses a major hurdle to effective treatment. Our inability to design novel drugs for antibiotic applications is in part due to a lack of understanding of the mechanisms of multi-drug resistance. This project will provide systems-level understanding of the operating principles governing how antibiotics are transported out of bacterial membranes by efflux pumps, dominant mechanism of drug resistance in many potential select-agent pathogens. The combined approach of multi-scale mathematical models and big data from large-scale simulations and high-throughput experiments proposed in this project is not limited to biological system, but rather can be applied to understand other multi-scale problems of interest to the Department of Energy(DOE)/ National Nuclear Security Administration(NNSA). It has the potential to connect the statistical physics based multi-scale models to high performance computing help solidify DOE's exascale computing initiatives, thereby strengthening the key NNSA goal of stockpile stewardship.

Technical Outcomes

The project successfully developed both machine learning (ML) models and microscopic models to account for and predict the active efflux and the outer membrane (OM) permeability barrier in Gram-negative bacteria. The mathematical model describes the bacterial colony from a bottom-up perspective providing insights on how microscopic inputs could impact macroscopic outcomes. The ML model predicts the permeation of compounds across the OM. Applications include to problems of interest to the Department of Energy (DOE).

Publications

Journal Articles

Manrique Charry, P. D., S. El Oud and N. Johnson. A Generalized Gelation Theory and the Growth of Online Extreme Communities. Submitted to *Nature Physics*. (LA-UR-20-25198)

Manrique Charry, P. D. and S. Gnanakaran. Microscopic Approach to Intrinsic Antibiotic Resistance. Submitted to *Nature Physics*. (LA-UR-20-27348)

Johnson, N., N. Velasquez, O. Jha, H. Niyazi, R. Leahy, N. Johnson Restrepo, R. Sear, P. D. Manrique Charry, Y. Lupu, P. Devkota, S. Wuchty and B. Goldberg. Covid-19 infodemic reveals new tipping point epidemiology and a revised R formula. Submitted to *Nature Human Behaviour*. (LA-UR-20-25193)

Velasquez, N., P. D. Manrique Charry, R. Sear, R. Leahy, N. Johnson Restrepo, L. Illary, Y. Lupu and N. Johnson. Hidden order across online extremist movements can be disrupted by nudging collective chemistry. Submitted to *Scientific Reports*. (LA-UR-21-21269)

Posters

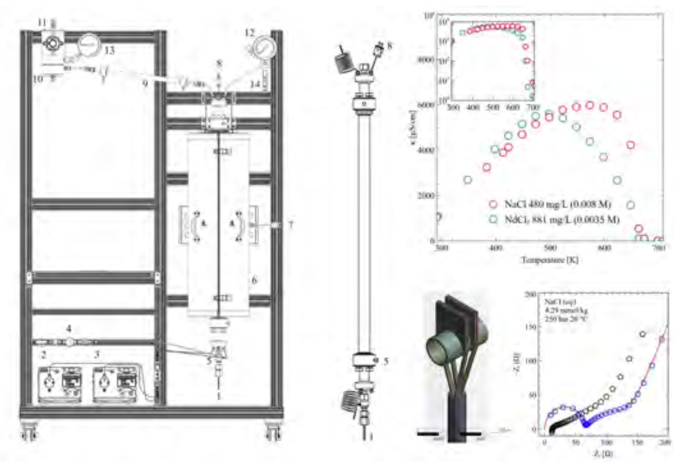
Manrique Charry, P. D., R. Henderson, S. Chakraborty, T. K. Nguyen, R. Mansbach, K. Wiehe, B. T. M. Korber and S. Gnanakaran. USING GRAPHS TO ANALYZE SARS-COV-2 MUTATIONS. Presented at *Biophysics Society Annual Meeting*, Boston, Massachusetts, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-21108)

Manrique Charry, P. D. and S. Gnanakaran. Multi-scale Antimicrobial Resistance Approach Featuring Cell-to-cell Heterogeneity Reveals Tradeoff Between Optimal Fitness and Colony Survival. Presented at *World Microbe Forum*, Virtual, New Mexico, United States, 2021-06-20 - 2021-06-24. (LA-UR-21-25653)

**Peer-reviewed*

Toward a Universal Description for Aqueous Solutions

Alp Findikoglu
20190653PRD4



In-situ characterization of high-temperature and high-pressure brines is technically challenging, but important to understand the geological processes in a laboratory setting, as well as to develop supercritical fluid processes for industrial applications. This project utilizes a continuous high-pressure flow unit equipped with a state-of-the-art in-situ electrochemical sensor, which is attached to a broadband frequency response analyzer. By analyzing the behavior in different electrolyte solutions (as pictured here), the flow unit will enable us to devise strategies to selectively recover certain salts from complex aqueous solutions.

Project Description

Meeting humanity's growing demand for fresh water is a major challenge. In particular, affordable methods to desalinate Earth's vast saline water resources remain elusive. One promising approach to meeting this challenge is supercritical water desalination, which is based on using high temperatures and pressures to manipulate water's properties and hence its ability to precipitate salts. Supercritical desalination is very well-suited for integration into other industrial processes; however, a number of both fundamental and practical issues exist. The proposed work combines both theoretical and experimental studies to make significant advances in our understanding of how salt ions and water behave in supercritical water. The knowledge generated by this work should have direct relevance for the development of the supercritical water desalination processes.

Technical Outcomes

Analytical, numerical, and experimental methods were developed to understand the behavior of salts in water at elevated temperatures and pressures. To interpret and predict electrical properties, different analytical models were developed and used to regress electrical properties obtained from experiments. The predicted electrical properties were then utilized to estimate the thermodynamic properties, which are essential for understanding supercritical water desalination processes. An open-ended coaxial probe technique and an in-situ conductometric sensor were also developed.

Publications

Journal Articles

Yoon, T. J., K. A. Maerzke, R. P. Currier and A. T. Findikoglu. PyOECP: A flexible open-source software library for estimating and modeling the complex permittivity based on the open-ended coaxial probe (OECP) technique. 2023. *Computer Physics Communications*. **282**: 108517. (LA-UR-21-29438 DOI: 10.1016/j.cpc.2022.108517)

*Yoon, T. J., L. A. Patel, T. Ju, M. J. Vigil, A. T. Findikoglu, R. P. Currier and K. A. Maerzke. Thermodynamics, dynamics, and structure of supercritical water at extreme conditions. 2020. *Physical Chemistry Chemical Physics*. **22** (28): 16051-16062. (LA-UR-20-22874 DOI: 10.1039/D0CP02288H)

Yoon, T., E. P. Craddock, J. C. Lewis, J. A. Matteson, J. Seong, R. P. Singh, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Supercritical water desalination with selective recovery of critical materials. Submitted to *Chemical Engineering Journal*. (LA-UR-21-30241)

Yoon, T., E. P. Craddock, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Electrical Conductances and association constants in dilute aqueous NdCl 3 solutions from 298 to 523 K along an isobar of 25 MPa. Submitted to *Journal of Chemical & Engineering Data*. (LA-UR-21-30907)

Yoon, T., E. Y. Raby, P. Sharan, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. Electrical characterization of binary mixtures and ternary nanostructured fluids composed of water, 2-propanol, and n-hexane. Submitted to *Journal of Molecular Liquids*. (LA-UR-20-30449)

Yoon, T., J. D. Riglin, P. Sharan, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. An in-situ conductometric apparatus for physicochemical characterization of solutions and in-line monitoring of separation processes at elevated temperatures and pressures. Submitted to *Measurement Science & Technology*. (LA-UR-21-29440)

*Yoon, T., M. J. Vigil, E. Y. Raby, R. P. Singh, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Dielectric relaxation of neodymium chloride in water and in methanol. 2020. *Journal of Molecular Liquids*. **308**: 112981. (LA-UR-19-32739 DOI: 10.1016/j.molliq.2020.112981)

Presentation Slides

Yoon, T., L. A. Patel, M. J. Vigil, A. T. Findikoglu, K. A. Maerzke and R. P. Currier. Understanding the Specific Conductance of NaCl Solutions in Water at Elevated Temperatures and Pressures. Presented at *2020 Virtual AIChE Annaul Meeting*, Los Alamos, New Mexico, United States, 2020-11-16 - 2020-11-20. (LA-UR-20-28738)

**Peer-reviewed*

Identifying Geometric Constraints Imposed by Antibiotics on Biomolecular Machines

Karissa Sanbonmatsu
20210759PRD1

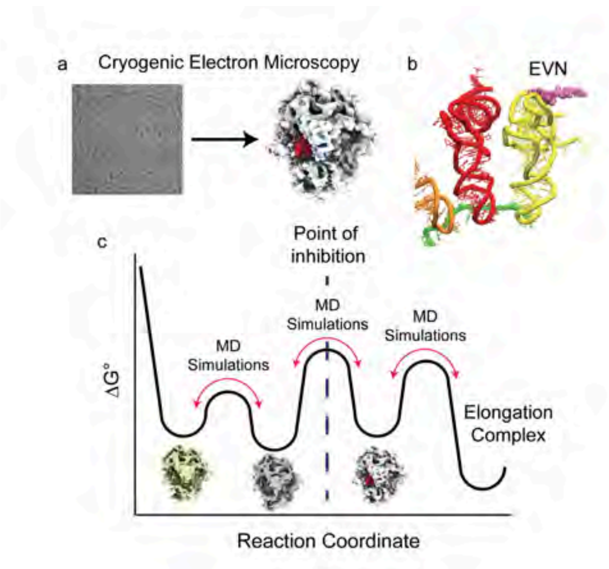


Figure 1. Structural dynamics of antibiotic dependent protein synthesis inhibition. (a) Cryogenic electron microscopy, (left) floated carbon grid with ribosomes in complex with mRNA, (right) 6.8 Å resolution structure of a ribosome (white) with mRNA (red). (b) Snap shot of evernimicin (EVN - pink) acting as a steric road block to the movement of the tRNA (yellow) into the ribosome. (c) Cryogenic electron microscopy resolved structures of ribosome complexes along the reaction coordinate of mRNA binding. MD simulations will be used to visualize the transition towards elongation complexes. Addition of antibiotics will reveal which structural dynamics of ribosomes are inhibited.

Project Description

The project outlined here focusses on the development of novel antibiotics for battling the looming threat of antimicrobial resistant pathogens. The current coronavirus (COVID-19) pandemic has shown how susceptible the global community is to a pandemic level threat. Resistant pathogens represent another pandemic level threat and with the lack of commercial interest in novel antibiotics it is critical that the public sector invest in their development. Development of novel antibiotics to combat pandemic level threats addresses the missions of biothreat as well as Pathogen Detection and Countermeasures. As resistant pathogens are becoming more common due to overuse and over prescription of antibiotics it is likely that they can be engineered. Using integrative electron microscopy and simulations approaches we aim to not only understand how conventional antibiotics work but provide a platform for the development and initial screening of novel antibiotics. This will help provide operational countermeasures against looming pathogenic threats.

Technical Outcomes

Molecular simulations of human ribosomes were performed to understand critical aspects of motion that differ between prokaryotes and eukaryotes. The main finding is that ribosomes have evolved to allow the transfer ribonucleic acid to have an additional degree of freedom during protein synthesis. The project team solved structures of the tetracycline class of antibiotics bound to the ribosomes using cryo-electron microscopy. This project improved understanding of antibiotic function to provide background for novel antibiotic development.

Publications

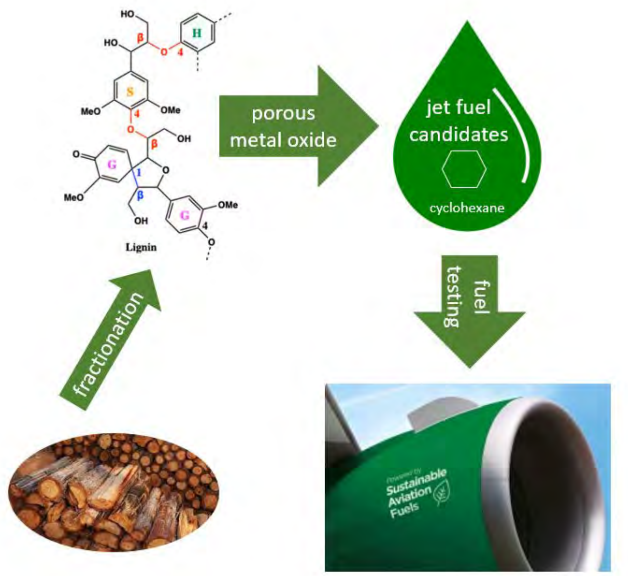
Posters

Girodat, D., H. Wieden, S. C. Blanchard and K. Y. Sanbonmatsu. Geometric alignment of aminoacyl-tRNA relative to catalytic centers of the ribosome underpins accurate mRNA decoding. Presented at *RNA Society*, Boulder, Colorado, United States, 2022-05-31 - 2022-06-05. (LA-UR-22-24094)

**Peer-reviewed*

Valorization of Lignin for the Production of High Performance Sustainable Aviation Fuels

Cameron Moore
20210762PRD1



Biomass derived fuels provide the potential to reduce greenhouse gas emissions and the foreign oil dependence in the United States. Researchers are tackling the challenges to synthesize sustainable aviation fuels (SAF) from biomass through thermochemical processes. Lignin and its abundant aromatic building blocks provide valuable resources to be upgraded to SAF blends. LDRD researchers are working to develop a low-cost, earth metal catalyst system to effectively convert lignin to SAF blends. Success with the copped doped porous metal oxide been synthesized so far, lignin model compounds are being studied in this catalytic system to test the catalyst performance in the lignin-to-SAF process.

Project Description

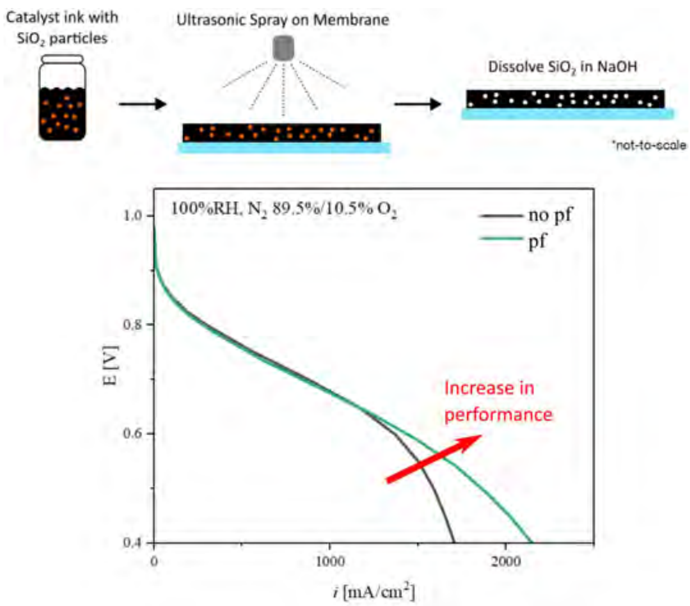
This project proposes to develop a scalable process for converting lignin from biomass into high performance aviation fuel. The project will include development of new chemistry as well as fuel testing to determine the suitability of the resulting products for aviation applications. This work will provide a basis for capturing the potential value of lignin which is often discarded or combusted. Valorization of lignin offers one potential route to enabling cost-competitive biofuels to enter the market and move the aviation industry toward their goal of reducing carbon dioxide (CO2) emissions by 2050. In addition, this work will help strengthen the nation's energy security by developing domestic production pathways for aviation fuel using agricultural waste products as feedstocks.

Technical Outcomes

This project aimed to develop an integrated process for the production of high-performance sustainable aviation fuel from biomass waste lignin. The team investigated pretreatment methods of soft woody biomass samples, lignin depolymerization approaches, and catalyst development for lignin hydrogenation. The new catalyst syntheses developed will enable further investigations in this field and application beyond biomass conversion.

Pore Size and Wettability of Control Electrodes for Next Generation Hydrogen Fuel Cells

Rangachary Mukundan
20210915PRD2



Sacrificial silica pore formers (pf) with known diameter are incorporated into the catalyst ink for hydrogen fuel cell applications. After catalyst ink deposition, the powders are dissolved away, leaving pores with controlled diameter. Preliminary experimental results reveal the benefits of controlled pores within the electrode for improved performance of hydrogen fuel cells.

Project Description

This study will demonstrate a powerful platform to better understand water transport in Polymer electrolyte membrane fuel cells (PEMFC) by developing a method for introducing controlled pore sizes into an electrode and tuning their wettability. Extensive characterization of the electrode structure and its performance as a fuel cell cathode will provide insights into the role of water management in increasing the utilization of platinum catalyst within the electrode. This project is expected to lead to design rules for the next generation of electrode that are not just random mixtures of porosity, catalyst, and ionic and electronic conducting phases. Since, the Platinum catalyst used in the electrode is the largest contributor (up to 53%) to the high cost of PEMFC systems, improved utilization of the catalyst can dramatically improve power density and decrease material costs. The results of this project will be applicable to other energy conversion devices like water and carbon dioxide (CO2), electrolyzers, and in desalination and hydrogen pumping applications.

Technical Outcomes

The goal of the project was to create a platform for controlling the wettability and the pore size of electrodes for fuel cells. As hypothesized, tuning the pore size distribution/porosity of the electrode had a significant effect on fuel cell performance. The project was successful in creating a design platform that could precisely control the pore size in the electrode.

Publications

Journal Articles

Lee, C. H., X. Wang, J. Peng, A. Katzenberg, R. K. Ahluwalia, A. Kusoglu, S. Komini Babu, J. S. Spendelow, R. Mukundan and R. L. Borup. Towards a Comprehensive Understanding of Cation Effects in Proton Exchange Membrane Fuel Cells. Submitted to *Joule*. (LA-UR-22-22836)

Lee, C., X. Wang, J. Peng, A. Katzenberg, R. Ahluwalia, A. Kusoglu, S. Komini Babu, J. S. Spendelow, R. Mukundan and R. L. Borup. Towards a Comprehensive Understanding of Cation Effects in Proton Exchange Membrane Fuel Cells. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-22-27788)

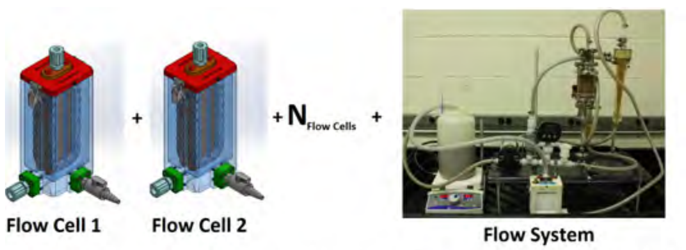
Lee, C., X. Wang, J. Peng, A. Katzenberg, R. Ahluwalia, A. Kusoglu, S. Komini Babu, J. S. Spendelow, R. Mukundan and R. L. Borup. Supporting Information: Toward a Comprehensive Understanding of Cation Effects in Proton Exchange Membrane Fuel Cells. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-22-27789)

Yang, G., C. H. Lee, X. Qiao, S. Komini Babu, U. Martinez and J. S. Spendelow. Advanced Electrode Structures for Proton Exchange Membrane Fuel Cells: Current Status and Path Forward. Submitted to *Advanced Materials*. (LA-UR-22-23045)

**Peer-reviewed*

Agile System for Electrochemical Dissolution of Bulk Actinide Oxides

Benjamin Karmiol
20210556MFR



The proposed LANL Modular Oxide Dissolution System (L-MODS) would provide new options for managing difficult to dissolve refractory materials in PF4. The system combines a customizable electrochemical flow-cell technology with an innovative flow system capable of suspending a wide variety of oxides. The electrochemical flow-cell technology is designed to make it easy to add or subtract electrochemical generation capacity as needed, and the flow system can accommodate various masses and types of materials. In additional, L-MODS does not require boiling the solution, eliminates the need for HF, and the solution is reusable, thus reducing TRU waste.

Project Description

Many actinide oxide bearing materials exist in the Department of Energy (DOE) complex. These materials often need to be stabilized for disposal or recovered for reuse. This can be achieved by burning the materials or dissolving and purifying the materials. Burning introduces certain risks (high energy, chemical reactions), and currently the only way to dissolve these materials is to use a boiling nitric acid fluoride ion solution which poses a high safety risk. The proposed research will develop a versatile electrochemical system that uses various catalysts to dissolve refractory actinide oxides, such as those described above. The system would allow for continuous reuse of the solution through electrolytic regeneration of the catalyst, elimination of fluoride ion, and dissolution at ambient temperatures. Testing will include determining rates of Plutonium Dioxide (PuO_2) dissolution using various catalysts. Information from these studies will allow for the design of a bulk actinide oxide dissolution systems that could be tailored (quantities of feed, types of feed, end-use of product, etc.) for low cost to meet dissolution needs. This project aims to develop customized actinide oxide dissolution options that could be deployed quickly, extending the capabilities of the Los Alamos Plutonium Facility (PF4).

Technical Outcomes

Los Alamos Modular Oxide Dissolution System (L-MODS) is an advanced plutonium oxide dissolution system which leverages additive manufacturing and modular design. Small-scale plutonium oxide dissolution studies using various catalysts have informed the design. A prototype system scaled for 1kilogram oxide capacity was tested using water and surrogate materials to demonstrate suspension of powders with varying characteristics. The electrochemical flow cell technology also advanced substantially to increase efficiency and ease of use in a glovebox.

Publications

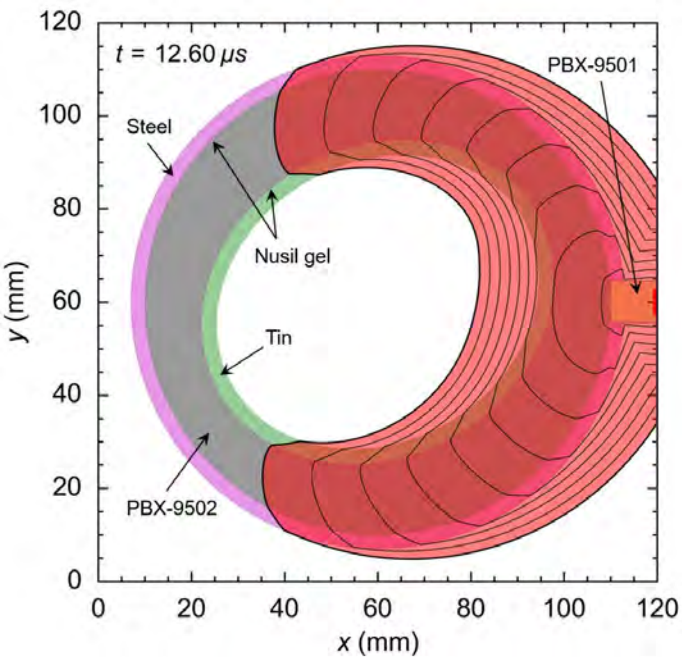
Presentation Slides

Karmiol, B., J. E. Droessler and S. P. Walsh. Agile System for Electrochemical Dissolution of Bulk Actinide Oxides (L-MODS). Presented at *LANL Weapon's Capability Review*, Los Alamos, New Mexico, United States, 2021-08-23 - 2021-08-26. (LA-UR-21-28202)

**Peer-reviewed*

Computational Modeling Tool for Rapid Performance Characterization of Novel High-explosive Design Geometries

Von Whitley
20210585MFR



The design of new high-explosive (HE) components involves many iterations and multi-physics models are resource-intensive. To expedite the process, researchers are developing a new computational tool capable of predicting the main HE performance features in seconds in a personal computer. The example depicted in the image (CYCLOPS) includes two different HEs and three inert materials. The calculation reproduces with good fidelity the experimental results and was completed in under 10 seconds on a 1900 x 1900 grid. The methodology also applies to 3D geometries which will contribute to an agile design process of complex HE components.

Project Description

Research into high explosives (HEs) has produced a number of innovations the past few years. New explosives molecules, newer and less sensitive formulations have been developed, and newer and faster manufacturing methods have been developed. All of the innovations need to be computationally evaluated to determine if they are acceptable for use in non-special nuclear material (SNM) nuclear explosive applications. The sheer number of innovations that need to be evaluated has overwhelmed the computational resources available. Thus adoption of these newer innovations is currently hindered by the computational time that is needed to evaluate the changes. This research proposed to produce a computational design tool that substantially speeds up the computational efficiency needed to evaluate new experimental designs. With these speed increases, we will be able to do initial design assessments using a single central processing unit (CPU) instead of thousands of nodes on a supercomputer. Other design studies that were impossible because they required more CPUs than the supercomputers currently contain, e.g., full three-dimensional (3D) design studies, will now be possible using our current supercomputers. Obtaining results in a matter of seconds on a personal computer will dramatically reduce the cost and time required in the design of HE components.

Technical Outcomes

This project accelerates our computational design studies by a factor of a million, reducing design time from a month-long endeavor to completion in seconds. The newly-devised models and algorithms lead to an engineering design tool capable of generating numerical simulations in seconds on a personal computer versus hours/days on High Performance Computing hardware. The ability to obtain rapid predictions of HE performance will directly assist Laboratory staff in the design and manufacturing of complex HE components.

Publications

Journal Articles

Lozano, E. and T. D. Aslam. Topological skeletons and local size of multidimensional objects using the fast sweeping method. Submitted to *Computers & Graphics*. (LA-UR-21-24854)

Tro, S. K., T. B. Mera Evans, T. D. Aslam, J. E. Lozano Sanchez and D. B. Culp. A second-order distributed memory parallel fast sweeping method for the Eikonal equation. 2022. *Journal of Computational Physics*. 111785. (LA-UR-22-31210 DOI: 10.1016/j.jcp.2022.111785)

Conference Papers

Lozano, E., T. D. Aslam, D. B. Culp and M. A. Price. Dynamic small resolved heat release model for programmed burn calculations. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*. (Anaheim, California, United States, 2022-07-11 - 2022-07-15). (LA-UR-22-31446)

Reports

Lozano, E. and T. D. Aslam. Taylor expansion wave solution for a general equation of state. Unpublished report. (LA-UR-22-27778)

Lozano, E. and T. D. Aslam. Fast Sweeping Detonation (FSD) model for programmed burn calculations. Unpublished report. (LA-CP-23-20163)

Presentation Slides

Lozano Sanchez, J. E., T. D. Aslam, D. B. Culp and M. A. Price. Dynamic small resolved heat release for programmed burn calculations. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26230)

Tro, S. K., T. B. Mera Evans, T. D. Aslam and J. E. Lozano Sanchez. Fast and Accurate Detonation Wave Calculations: A Second Order Distributed Memory Parallel Fast Sweeping Method For the Eikonal Equation. Presented at *XCP Summer Student talks*, Los Alamos, New Mexico, United States, 2022-08-18 - 2022-08-18. (LA-UR-22-28640)

Posters

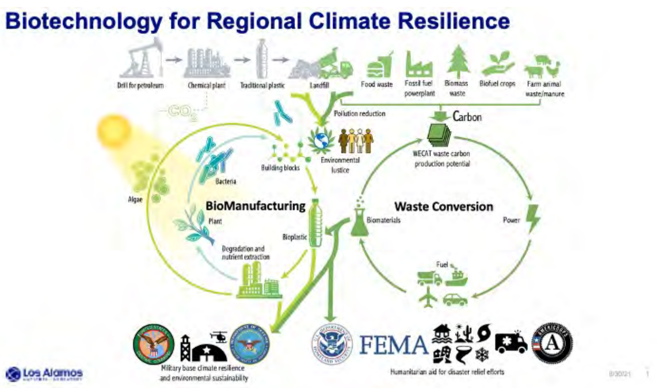
Tro, S. K., T. B. Mera Evans, T. D. Aslam and J. E. Lozano Sanchez. Fast and Accurate Detonation Wave Calculations: A Second Order Distributed Memory Parallel Fast Sweeping Method For the Eikonal Equation. . (LA-UR-22-28348)

Whitley, V. H. and C. A. DeBurgomaster. Select Hugoniot Curves and Materials Data. . (LA-UR-21-30934)

**Peer-reviewed*

Biotechnology for Regional Climate Resilience

Babetta Marrone
20210921DI



The project will enable local climate resilience and mitigation goals with innovative tools and technologies that will help develop sustainable, biological solutions to critical needs for energy and materials in fixed or mobile military operations, and surrounding communities. In the left circle is a typical biomanufacturing loop where biomass or microorganisms are used to produce materials or chemicals that replace current products made from petroleum. The right circle shows the WECAT tool (Waste-carbon Economic and Climate Action Tool), for identifying waste carbon sources that can be utilized by a military base or other operations to generate power, fuels, or tactical biomaterials.

Project Description

With a changing climate comes risks associated with extreme heat, fire, drought, floods, hurricanes, and other climate and weather-related events. This project aims to develop tools and technologies to meet local to regional climate resilience and mitigation objectives with a focus on military applications: stationary bases; forward operating bases; and Humanitarian Assistance and Disaster Relief operations. Our aim is to develop tools and technologies to promote the use of waste carbon, including carbon dioxide, food waste, and plastics, to improve the environmental sustainability of military operations during climate and weather-related disasters. Our first goal is to create a new climate action geospatial tool that can be used to predict local- to country-scale potential for waste carbon development into desirable products (e.g. energy, water, biomaterials, fuel). Our second goal is to develop a biomanufacturing technology to convert waste carbon to usable products (building and construction materials, fuels). Our project will lay the groundwork to develop sustainable, biological solutions to critical needs for energy and materials in fixed or mobile military operations that enable adaptation and agility in response to challenges of climate change and extreme weather events.

Technical Outcomes

A data-driven, geospatial model was constructed to determine the portfolio of energy resources at the national scale and optimized according to greenhouse gas and monetary cost reduction. The model includes a prototype web interface to access and visualize data, optimization parameters, and results. Biomanufacturing focused on mechanical performance of cement embedded with pozzolanic and microalgae materials. Pozzolanic fillers increased the compressive strength of the cement. Algae addition decreased the compressive strength, and increased porosity.

Publications

Reports

Mejia Castro, B. M. and J. E. Barefield. LIBS Spectral Data. Unpublished report. (LA-UR-22-32926)

Presentation Slides

Atencio, A. D., M. M. Hernandez and J. H. Dumont. Microscopy images of Spirulina Platensis. . (LA-UR-21-31002)

Dale, T. T. Bio-based solutions to transform the climate and clean energy systems. . (LA-UR-22-32234)

Gonzalez Esquer, C. R. Direct air capture of CO2 for supporting for supporting algae growth on ePBRs. . (LA-UR-23-20685)

Hernandez, M. M., A. D. Atencio, C. R. Gonzalez Esquer, B. L. Marrone and J. H. Dumont. Algae and Concrete Composites: Structural Materials as a CO2 sink. Presented at *ACS Fall 2021 Meeting*, Boston, Massachusetts, United States, 2021-11-29 - 2021-12-02. (LA-UR-21-31590)

Hernandez, M. M., B. M. Mejia Castro, C. R. Gonzalez Esquer, B. L. Marrone and J. H. Dumont. Use of Waste Bioproducts as a CO2 Sink in Sustainable Structural Composites. Presented at *New Mexico Research Symposium*, Albuquerque, New Mexico, United States, 2022-11-05 - 2022-11-05. (LA-UR-22-31748)

Marrone, B. L. Bio-based Solutions for Climate Resilience, Clean Energy, and Carbon Neutrality. . (LA-UR-22-29853)

Marrone, B. L. and C. R. Gonzalez Esquer. Algae Biomanufacturing to Enable a Circular Carbon Economy in the Intermountain West. Presented at *Algae Biomass Summit*, Virtual Los Alamos, New Mexico, United States, 2022-10-03 - 2022-10-28. (LA-UR-22-30819)

Posters

Mejia Castro, B. M., M. M. Hernandez, C. R. Gonzalez Esquer, B. L. Marrone and J. H. Dumont. Hydrogels as a Support Medium for the Culture of Cyanobacteria. Presented at *New Mexico research Symposium*, Albuquerque, New Mexico, United States, 2022-11-05 - 2022-11-05. (LA-UR-22-31669)

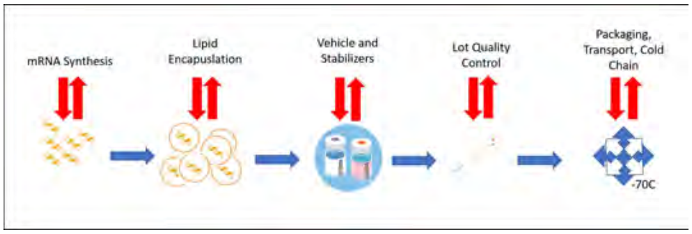
Gonzalez Esquer, C. R., A. R. Witt, M. M. Hernandez, J. H. Dumont and B. L. Marrone. Alginate Hydrogels and Cyanobacterial Composites as Renewable Biomaterials. . (LA-UR-22-27998)

Hernandez, M. M., A. R. Witt, Y. Trujillo, C. R. Gonzalez Esquer, B. L. Marrone and J. H. Dumont. Use of Waste Bioproducts as a CO2 Sink in Sustainable Structural Composites. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27695)

**Peer-reviewed*

Understanding the Risks and Mitigation Strategies in Securing Vaccine Biomanufacturing Processes

Jennifer Harris
20220615DI



The vaccine manufacture process is largely automated from production to quality control, to packaging and transport. Red arrows denote software input into the process where computer-based instructions are provided to automated equipment and the equipment reports back to the computers running the system. The disruption of one or more of these processes could result in severe damage to the vaccine supply chain .

Project Description

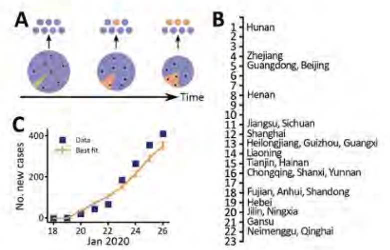
The team proposes performing a cybersecurity assessment of vaccine manufacturing workflows and manufacturing processes. Strengths and weaknesses of the automated vaccine manufacture process will be identified so that any vulnerabilities can be mitigated immediately. This will help assure public trust in our medical system by helping keep the vaccine supply safe. In this work the team will assess vaccine research and development, manufacturing, quality control, distribution, hiring practices and tracking the effects of vaccines post deployment. During the course of the assessment the team will make use of ontological modeling approaches to model the vaccine deployment chain for further technical assessments.

Technical Outcomes

The project team developed software called BioMan to quantify risk in process steps of biomanufacturing, The project built a prototype of this tool to 1) describe the different components of a biomanufacturing process, 2) to model the interdependencies across process components, and 3) to simulate the nonlinear cascading effects of a perturbation of the process to estimate the risks associated with perturbation.

Mechanistic Studies of Human Disease

Nicolas Hengartner
20200002CR-CNL



Estimates of the exponential growth rate and the date of exponential growth initiation of the outbreak in China. A) Export of infected persons from Wuhan. Because of the growth of the infected population (orange pie) and the shrinking size of the total population over time, probability of infected persons traveling to other provinces increases (orange dots). B) The dates of documented first arrivals of infected persons in 26 provinces. C) Best fit of the case count model to daily counts of new cases in provinces other than Hubei. Fig. 3 from Sanche et al. Emerging Infectious Diseases,26, 2020.

Project Description

This project aims at modeling biological systems using computational and mathematical methods. Biological systems are modeled at different scales: atomistic (proteins, nuclei acids in various environments), systems of proteins described as members of an interacting (biochemical network), and dynamical non-linear systems that can show interesting behaviors in response to small perturbations. These models are used to model diseases and, potentially, to design new drugs that target specific proteins. The research is done in interdisciplinary teams that include biologists, physicists, and mathematicians. Postdoctoral fellows conduct the research under the supervision of Laboratory staff scientists. The modeling of signaling pathways related to cancer align with the Department of Energy's interest in developing high-performance computing and modeling approaches to help diagnose cancer patients. The development of new computational and modeling capability to study biomembranes will be relevant to health and biotechnology applications.

Technical Outcomes

This project contributed to the long-term scientific vitality of Los Alamos bioscience capability and developed new capability in computational biology and epidemic modeling. The research also supported the laboratory's nimble engagement on Coronavirus disease (COVID) research.

Publications

Journal Articles

*Berndsen, Z. T., S. Chakraborty, X. Wang, C. A. Cottrell, J. L. Torres, J. K. Diedrich, C. A. L\xc3\xb3pez, J. R. Yates, M. J. van Gils, J. C. Paulson, S. Gnanakaran and A. B. Ward. Visualization of the HIV-1 Env glycan shield across scales. 2020. *Proceedings of the National Academy of Sciences*. **117** (45): 28014-28025. (LA-UR-19-30964 DOI: 10.1073/pnas.2000260117)

Brunner, J. D. and N. Chia. Metabolic Model-based Ecological Modeling for Probiotic Design. Submitted to *eLife*. (LA-UR-22-30397)

*Castro, L. A., N. Generous, W. Luo, A. Pastore y Piontti, K. Martinez, M. F. C. Gomes, D. Osthus, G. Fairchild, A. Ziemann, A. Vespignani, M. Santillana, C. A. Manore and S. Y. Del Valle. Using heterogeneous data to identify signatures of dengue outbreaks at fine spatio-temporal scales across Brazil. 2021. *PLOS Neglected Tropical Diseases*. **15** (5): e0009392. (LA-UR-20-29637 DOI: 10.1371/journal.pntd.0009392)

Chakraborty, S., Z. T. Berndsen, N. W. Hengartner, B. T. M. Korber, A. B. Ward and S. Gnanakaran. Quantification of the Resilience and Vulnerability of HIV-1 Native Glycan Shield at Atomistic Detail. Submitted to *iScience (Cell Press)*. (LA-UR-19-30981)

*Cuellar, L., I. Torres, E. Romero-Severson, R. Mahesh, N. R. Ortega, S. A. Pungitore, N. W. Hengartner and R. Ke. Excess deaths reveal the true spatial, temporal and demographic impact of COVID-19 on mortality in Ecuador. 2021. *International Journal of Epidemiology*. (LA-UR-21-21361 DOI: 10.1093/ije/dyab163)

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Fox, Z. R. Extracting Trajectories from Stochastic Trajectories of Gene Expression. Submitted to *Physical Review Letters*. (LA-UR-22-21680)

*Fox, Z. R., E. Barkai and D. Krapf. Aging power spectrum of membrane protein transport and other subordinated random walks. 2021. *Nature Communications*. **12** (1): 6162. (LA-UR-21-21176 DOI: 10.1038/s41467-021-26465-8)

Fox, Z. R., S. Fletcher, A. Fraisse, C. Aditya, S. Sosa-Carrillo, S. Gilles, F. Bertaux, J. Ruess and G. Batt. MicroMator: Open and Flexible Software for Reactive Microscopy. Submitted to *Nature Methods*. (LA-UR-21-22416)

*Janke, J. J., Y. Yu, V. H. Pomin, J. Zhao, C. Wang, R. J. Linhardt and A. E. Garcia. Characterization of Heparin's Conformational Ensemble by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Spectroscopy. 2022. *Journal of Chemical Theory and Computation*. **18** (3): 1894-1904. (LA-UR-20-28381 DOI: 10.1021/acs.jctc.1c00760)

Ke, R., S. Sanche, E. Romero-Severson and N. W. Hengartner. Fast spread of COVID-19 in Europe and the US and its implications: even modest public health goals require comprehensive intervention. Submitted to *Lancet Infectious Diseases*. (LA-UR-20-22635)

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*Mansbach, R. A., T. Travers, S. Chakraborty and S. Gnanakaran. Graph-Directed Approach for Downselecting Toxins for Experimental Structure Determination. 2020. *Structure*. **18** (5): 256. (LA-UR-19-26210 DOI: 10.3390/md18050256)

Meyers, K., L. Liu, W. W. Lin, Y. Luo, M. T. Yin, Y. Wu, S. N. Wontakal, F. La Carpia, S. Fernando, M. Dowlatshahi, L. Joshua-Tor, J. Wolk, B. Alpert, M. Romney, B. K. Costabile, E. L. Gelardi, F. Vallese, O. B. Clarke, F. Mancia, A. Uhlemann, M. Sobiezczyk, A. S. Perelson, Y. Huang, E. A. Hod and D. D. Ho. Antibody Testing Documents the Silent Spread of SARS-CoV-2 in New York Prior to the First Reported Case. Submitted to *New England Journal of Medicine*. (LA-UR-20-23502)

*Migliori, A. D., L. A. Patel and C. Neale. The RIT1 C-terminus associates with lipid bilayers via charge complementarity. 2021. *Computational Biology and Chemistry*. **91**: 107437. (LA-UR-19-32749 DOI: 10.1016/j.compbiolchem.2021.107437)

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**Peer-reviewed*

Information Science and Technology

Uncertainty Quantification for Robust Machine Learning

Diane Oyen

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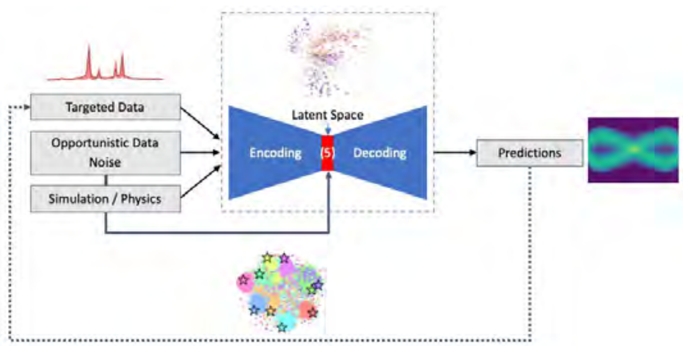

The Uncertainty Quantification for Robust Machine Learning (UQ4ML) project aims to develop methods that jointly evaluate uncertainties at the input, latent space, and output layers of machine learning models. The project includes closing the loop to inform future data collection choices based on the overall value of new (and potentially heterogenous) data sources.

Project Description

This project will develop uncertainty quantification tools needed to verify and validate artificial intelligence models for high stakes scientific applications. Assurance is one of the most challenging problems facing artificial intelligence (AI). Assurance addresses the question of whether an AI model has been constructed, trained, and deployed so that it is appropriate for its intended use. Building such assured AI models for science problems is complex because science is evolutionary where scientists often recycle past data and models. Training machine learning models on data produced by simulations invariably omits both the complexities and the subtle statistical patterns of real-world science datasets. This project will advance our understanding of quantifying uncertainty in machine learning (ML) and developing the needed software tools to apply ML to the challenges of mission-critical science and security problems.

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Posters

Castorena, J. E. and D. A. Oyen. SpectroscopyNet: Learning to pre-process spectroscopy signals without clean data. Presented at *56th Annual Asilomar Conference on Signals, Systems, and Computers*, Monterey, California, United States, 2022-10-30 - 2022-11-04. (LA-UR-22-29564)

Geyer, M. A., B. W. Bell, A. Fernandez and J. S. Moore. Practical Path Kernels: Approximating Neural Networks as Kernel Machines. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-10. (LA-UR-23-22237)

Geyer, M. A. and J. S. Moore. Exploring Saliency Metrics of Radio Frequency Data. Presented at *Naval Applications in Machine Learning*, San Diego, California, United States, 2023-03-20 - 2023-03-24. (LA-UR-23-22827)

Jones, H. T., J. M. Springer, G. Kenyon and J. S. Moore. If You\xc3\xa2 Trained One You\xc3\xa2 Trained Them All. Presented at *UC Riverside Security and Autonomy Workshop*, Riverside, California, United States, 2022-06-02 - 2022-06-02. (LA-UR-22-24986)

Jones, H. T., J. M. Springer, G. Kenyon and J. S. Moore. If You’ve Trained One You’ve Trained Them All. Presented at *Conference on Uncertainty in Artificial Intelligence (UAI) 2022*, Eindhoven, Netherlands, 2022-08-01 - 2022-08-05. (LA-UR-22-26385)

Jones, H. T. and J. S. Moore. Is the Discrete VAE’s Power Stuck in its Prior?. Presented at *1st I Can’t Believe It’s Not Better Workshop (ICBINB@NeurIPS 2020)*, Online, New Mexico, United States, 2020-12-12 - 2020-12-12. (LA-UR-20-30005)

Klein, N. E., N. Panda, P. J. Gasda and D. A. Oyen. Generative structured normalizing flow Gaussian processes applied to spectroscopic data. Presented at *AAAI Conference on Artificial Intelligence*, Online, Canada, 2022-02-22 - 2022-02-22. (LA-UR-22-21243)

Kucer, M., D. A. Oyen and G. Kenyon. When does visual self-supervision aid adversarial training in improving adversarial robustness. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*, New Orleans, Louisiana, United States, 2022-11-28 - 2022-12-09. (LA-UR-22-32620)

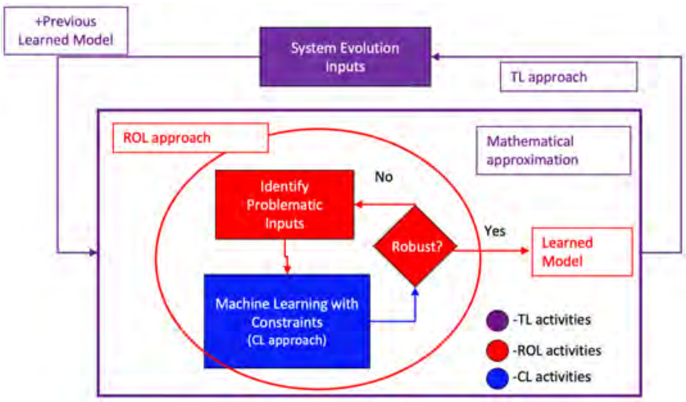
Oyen, D. A., M. Kucer, N. W. Hengartner and H. S. Singh. Robustness to Label Noise Depends on the Shape of the Noise Distribution. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*, New Orleans, Louisiana, United States, 2022-11-28 - 2022-11-28. (LA-UR-22-32068)

Poshiya, S. K. and M. Kucer. Exploring Representations Learned from Image Transformations as Pretext Tasks. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27758)

**Peer-reviewed*

The Optimization of Machine Learning: Imposing Requirements on Artificial Intelligence

Russell Bent
20210078DR



The core of the machine learning is an optimization solver (constrained learning (CL)) that expresses constraints as part of the learning (blue). The robust learning, ROL, (red) is an algorithm which efficiently and iteratively identifies problematic inputs for the training set—each iteration of the ROL algorithm uses CL to train a new model (red text). In real-time environments, the tractable learning, TL, (purple) derives computationally efficient approximations which have computable error bounds.

Project Description

By advancing and synthesizing the areas of machine learning (ML), this project integrates areas of that are central to Department of Energy (DOE) and Los Alamos National Laboratory (LANL) science and mission needs. In areas as diverse as non-proliferation, materials, and complex engineered systems, emerging DOE challenges are an outcome of larger and larger volumes of complicated data, for which it is natural to suggest ML as a solution. However, DOE analyses in these areas are mission critical and have high consequences for failure, and hence require high confidence ML solutions. We identify the core information sciences problems that are directly relevant for high-consequence DOE decision making and devise novel efficient constrained machine learning algorithms with robustness and efficiency guarantees. Through a unique and strong collaboration between top optimization, machine learning, and domain scientists at LANL, we develop a novel machine learning paradigm that combines constrained optimization, robust optimization, and tractability with machine learning to meet key Information Science & Technology (IS&T) challenges. The applied value of this research is demonstrated by sharpening the solutions for problems in ground feature detection and complex engineered energy systems.

Publications

Journal Articles

Andresen, C. and E. S. Schultz-Fellenz. The use of UAS photogrammetry to advance the spatial and temporal frontiers of change detection in the earth sciences. Submitted to *Earth-Science Reviews*. (LA-UR-22-24049)

*Chertkov, M., V. Chernyak and Y. Maximov. Gauges, loops, and polynomials for partition functions of graphical models. 2020. *Journal of Statistical Mechanics: Theory and Experiment*. **2020** (12): 124006. (LA-UR-20-30432 DOI: 10.1088/1742-5468/abcaf0)

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Deka, D., h. doddi, S. Misra and M. Salapaka. Tractable learning in under-excited power grids. Submitted to *IEEE Transactions on Control of Network Systems*. (LA-UR-21-29122)

Deka, D., m. bariya and A. von Meier. Guaranteed Phase & Topology Identification in Three Phase Distribution Grids. Submitted to *IEEE Transactions on Smart Grid*. (LA-UR-22-32190)

Deka, D., r. wang, M. R. A. Paternina and W. Li. Physics-Constrained Adversarial Training for Neural Networks in Stochastic Power Grids. Submitted to *IEEE Transactions on Artificial Intelligence*. (LA-UR-23-20922)

Delabays, R., A. Lokhov, M. S. Tyloo and M. D. Vuffray. Locating the source of forced oscillations in transmission power grids. Submitted to *Nature Energy*. (LA-UR-22-32412)

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Hijazi, H. L., S. Gopinath, A. M. A. Hijazi, J. B. Dann, A. D. Collins, E. S. Schultz-Fellenz, R. W. Bent, G. Riemersma and N. W. Lemons. Globally Optimal Boresight Alignment of UAV-LiDAR Systems. Submitted to *IEEE Transactions on Multimedia*. (LA-UR-20-28088)

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Lukashevich, A., V. Gorchakov, P. Vorobev, D. Deka and Y. Maximov. Importance Sampling Approach to Chance-Constrained DC Optimal Power Flow. Submitted to *Elsevier EPSR*. (LA-UR-21-31757)

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Misra, S., K. Sundar, R. Sharma and K. Brink. Deployable, Data-Driven Unmanned Vehicle Navigation System in GPS-Denied, Feature-Deficient Environments. Submitted to *Journal of Intelligent and Robotic Systems*. (LA-UR-21-20249)

*Snyder, J., A. Zlotnik and A. Y. Lokhov. Data-driven selection of coarse-grained models of coupled oscillators. 2020. *Physical Review Research*. **2** (4): 043402. (LA-UR-20-27371 DOI: 10.1103/PhysRevResearch.2.043402)

Sundar, K., S. Sanjeevi and H. Nagarajan. Sequence of polyhedral relaxations for nonlinear univariate functions. 2022. *Optimization and Engineering*. **23** (2): 877-894. (LA-UR-20-23980 DOI: 10.1007/s11081-021-09609-z)

Turan, E. M., J. Jaschke and R. Kannan. Optimality-Based Discretization Methods for the Global Optimization of Nonconvex Semi-Infinite Programs. Submitted to *Mathematical Programming*. (LA-UR-23-22257)

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Bent, R. W., B. A. Tasseff and C. J. Coffrin. INFRASTRUCTUREMODELS: Composable Multi-Infrastructure Modeling in Julia. Presented at *Power Systems Computation Conference*. (Porto, Portugal, 2022-06-27 - 2022-06-27). (LA-UR-21-29947)

Bent, R. W., C. J. Coffrin and B. A. Tasseff. Modeling Electric Power Systems and Interdependencies with Natural Gas and Water: An Optimization Software Solution. Presented at *Power Systems Computation Conference*. (Porto, Portugal, 2022-06-27 - 2022-06-27). (LA-UR-21-29852)

Burashnikova, A., Y. Maximov, M. Clausel, C. Laclau, F. Iutzeler and M. R. Amini. Learning over No-Preferred and Preferred Sequence of Items for Robust Recommendation (Extended Abstract). Presented at *IJCAI (International Jount Conference on Artificial Intelligence)*. (Vienna, Austria, 2022-07-01 - 2022-07-08). (LA-UR-22-22124)

Cengil, M. F., H. Nagarajan, R. W. Bent, S. Eksioglu and B. Eksioglu. Learning to Accelerate Globally Optimal Solutions to the AC Optimal Power Flow Problem. Presented at *Power Systems Computation Conference*. (Porto, Portugal, 2022-06-27 - 2022-07-01). (LA-UR-21-30785)

Deka, D., W. Li, M. Kamal and H. Mohsenian-Rad. Physics-Conditioned Generative Adversarial Networks for State Estimation in Active Power Distribution Systems with Low Observability. Presented at *International Conference on Smart Grid Synchronized Measurements and Analytics*

(SGSMA). (Split, Croatia, 2022-05-24 - 2022-05-26). (LA-UR-22-32187)

Dutt, A., A. Lokhov, M. D. Vuffray and S. Misra. Exponential Reduction in Sample Complexity with Learning of Ising Model Dynamics. Presented at *International Conference on Machine Learning (ICML)*. (Online, New Mexico, United States, 2021-07-18 - 2021-07-24). (LA-UR-21-21523)

Hannon, C., D. Deka, D. Jin, M. D. Vuffray and A. Lokhov. Real-time Anomaly Detection and Classification in Streaming PMU Data. Presented at *IEEE PowerTech 2021*. (Online, New Mexico, United States, 2021-06-28 - 2021-06-28). (LA-UR-22-31538)

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Li, W., D. Deka and D. Krishnamurthy. Physics-Constrained Interval Bound Propagation for Robustness Verifiable Neural Networks in Power Grids. Presented at *AI for Energy Innovation, AAAI Conference on Artificial Intelligence*. (Washington, District Of Columbia, United States, 2023-02-07 - 2023-02-14). (LA-UR-23-20362)

Li, W., K. Dvijotham and D. Deka. Physics-Constrained Interval Bound Propagation for Robustness Verifiable Neural Networks in Power Grids. Presented at *Workshop (W4): AI for Energy Innovation held in conjunction with 37th AAAI Conference on Artificial Intelligence (AAAI-23)*. (Washington, District Of Columbia, United States, 2023-02-13 - 2022-12-13). (LA-UR-23-20187)

Lokhov, A., S. Misra, C. X. Ren and M. D. Vuffray. Learning Continuous Exponential Families Beyond Gaussian. Presented at *International Conference on Machine Learning (ICML)*. (Online, New Mexico, United States, 2021-07-18 - 2021-07-24). (LA-UR-21-21520)

Misra, S., M. D. Vuffray and A. Lokhov. Information Theoretic Optimal Learning of Gaussian Graphical Models. Presented at *Conference on Learning Theory*. (Online, New Mexico, United States, 2020-07-09 - 2020-07-09). (LA-UR-20-24929)

Ren, C. X., S. Misra, M. D. Vuffray and A. Lokhov. Learning Continuous Exponential Families Beyond Gaussian. Presented at *NeurIPS 2022*. (New Orleans, Louisiana, United States, 2022-11-28 - 2022-11-28). (LA-UR-22-25979)

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *NeurIPS 2020*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-25018)

Reports

Amini, M. R., V. Feofanov, L. Pauletto, E. Devijver and Y. Maximov. Self-Training: A Survey. Unpublished report. (LA-UR-22-21924)

Burashnikova, A., M. Clausel, C. Laclau, F. Iutzeler, Y. Maximov and M. Amini. Learning over no-Preferred and Preferred Sequence of Items for Robust Recommendation. Unpublished report. (LA-UR-20-30431)

Burashnikova, A., M. Clausel, M. R. Amini, N. Dante and Y. Maximov. Recommender systems : when memory matters. Unpublished report. (LA-UR-21-31786)

Burashnikova, A., M. R. Amini, D. Deka, W. Li and Y. Maximov. Ranking-Based Physics-Informed Line Failure Detection in Power Grids. Unpublished report. (LA-UR-22-29132)

Lokhov, A. and M. D. Vuffray. Advanced AI solutions for locating forced oscillations in critical infrastructures. Unpublished report. (LA-UR-21-32165)

Lukashevich, A. and Y. Maximov. Power Grid Reliability Estimation via Adaptive Importance Sampling. Unpublished report. (LA-UR-21-22685)

Lukianenko, I., M. Mosikov, I. Makarov and Y. Maximov. Long-Term Hail Risk Assessment with Deep Neural Networks. Unpublished report. (LA-UR-22-29120)

Mitrovic, M., A. Lukashevich, P. Vorobev, V. Terzija, S. Budenny, Y. Maximov and D. Deka. Data-Driven Stochastic AC-OPF using Gaussian Process Regression. Unpublished report. (LA-UR-22-28238)

Mitrovic, M., A. Lukashevich, P. Vorobev, V. Terzija, Y. Maximov and D. Deka. Data-Driven Chance Constrained AC-OPF using Hybrid Sparse Gaussian Processes. Unpublished report. (LA-UR-22-29131)

Mitrovic, M., D. Deka, P. Vorobev and Y. Maximov. Data-Driven Stochastic AC-OPF using Gaussian Processes. Unpublished report. (LA-UR-22-21807)

Sidana, S., M. Trofimov, O. Horodnitskii, C. Laclau, Y. Maximov and M. R. Amini. User Preference and Embedding Learning with Implicit Feedback for Recommender Systems. Unpublished report. (LA-UR-20-30410)

Presentation Slides

Bent, R. W., S. Misra, H. Nagarajan, D. Deka, C. J. Coffrin and H. L. Hijazi. AI4Opt Collaboration Discussion. . (LA-UR-22-30755)

Cengil, F., H. Nagarajan, R. W. Bent, S. Eksioglu and B. Eksioglu. Learning to Accelerate Globally Optimal Solutions to the AC Optimal Power Flow Problem. Presented at *Grid Science Winter School and Conference*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-13. (LA-UR-23-20113)

Coffrin, C. J. A Brief Introduction to Mathematical Optimization in Julia (Part 1). Presented at *2021 Grid Science Winter School & Conference*, Los Almos, New Mexico, United States, 2021-01-11 - 2021-01-15. (LA-UR-21-20278)

Dutt, A., M. D. Vuffray, A. Lokhov and S. Misra. Exponential Reduction in Sample Complexity with Learning of Ising Model Dynamics. Presented at *Information Theory and Application Workshop 2022*, San Diego, California, United States, 2022-05-22 - 2022-05-27. (LA-UR-22-24703)

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Goutham, M., R. Kannan, H. Nagarajan and D. Deka. Electricity Grid Resilience: Preventing the next Blackout. . (LA-UR-22-28780)

Goutham, M., R. Kannan, H. Nagarajan and D. Deka. Electricity Grid Resilience: Preventing the next Blackout. . (LA-UR-22-28944)

Kannan, R., D. Deka and H. Nagarajan. Learning to Accelerate the Global Solution of Quadratically-Constrained Quadratic Programs. Presented at *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Phoenix, Arizona, United States, 2022-11-13 - 2022-11-13. (LA-UR-22-31958)

LaRochelle, G. R. LIDAR Analytics for National Security: Workflow Creation and Capability Exploration. . (LA-UR-22-28378)

Lee, J. E., H. L. Hijazi, S. Gopinath, A. D. Collins, B. M. Crawford, E. S. Schultz-Fellenz and R. W. Bent. Machine Learning 4 Optimization: Applications for DoE-EM-TDO IAA. Presented at *DoE Env. Manag. Tech. Dev. Office Interagency Agreement*, Online, New Mexico, United States, 2022-06-16 - 2022-06-16. (LA-UR-22-25642)

Lokhov, A. Physics-Inspired Machine Learning and Data Analytics for Energy Systems. . (LA-UR-21-22541)

Lokhov, A. Real-time Anomaly Detection and Classification in Streaming PMU Data. Presented at *PowerTech 2021*, Madrid, Spain, 2021-06-28 - 2021-06-28. (LA-UR-21-26132)

Lokhov, A. Locating the source of forced oscillations in transmission power grids. Presented at *Grid Science Winter School and Conference*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-09. (LA-UR-23-20309)

Maximov, Y. Impactful Rare Event: Theory & Practice. . (LA-UR-22-27597)

Milazzo, D. M. LAGS 2023 - Earth and Planetary Sciences UAS Capabilites, Programmatic Successes, and Future Endeavors. Presented at *Los ALamos Geological Society Monthly Meeting*, Los Alamos, New Mexico, United States, 2023-03-21 - 2023-03-21. (LA-UR-23-22857)

Schultz-Fellenz, E. S. Applied ML Needs in Uncrewed Aerial Systems. . (LA-UR-22-21378)

Tasseff, B. A. Optimization of Critical Infrastructure with Fluids. . (LA-UR-21-26827)

Wilinski, M. J. and A. Lokhov. Network Reconstruction from Noisy and Incomplete Spreading Dynamics. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22253)

Posters

Coats, D. E., D. Delparte, T. Calton, T. T. Caughlin, E. S. Schultz-Fellenz and J. S. Forbey. Analyzing the Relationship Between Land Use and Land Cover Trends and Columbian Sharp-tailed Grouse Lekking Populations in Southeastern Idaho. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32472)

Goutham, M., R. Kannan, D. Deka, H. Nagarajan and R. W. Bent. Optimal Power Flow for Resilient Electric Grids under Uncertain Hurricane Forecasts: A Multi-Stage Stochastic Programming Approach. Presented at *2023 Grid Science Winter School and Conference*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-13. (LA-UR-23-20059)

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**Peer-reviewed*

Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems

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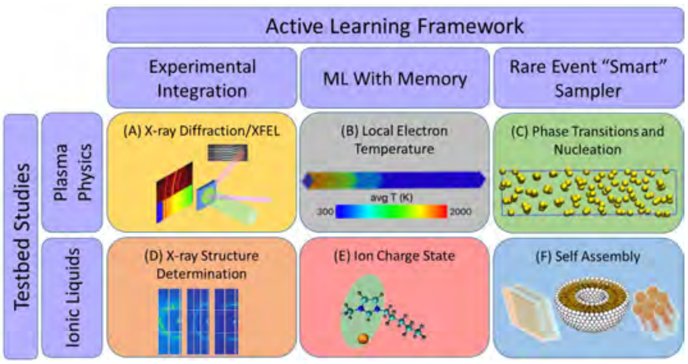
20210087DR



The main goal of this project is the development of an Active Learning Framework (ALF) capable of automatically constructing machine learned (ML) interatomic potentials for both metallic and soft matter systems. The developed framework will be tested on two distinct experimental applications: Shocked metals and self-assembly of ionic liquids. The ALF framework will incorporate a variety of advancements to ML potentials including the ability to train to experimental data, incorporation of supplementary variables such as electronic temperature and atomic charge, and intelligent sampling schemes.

Project Description

This work seeks to develop new, more accurate, atomic models for the behavior of aged materials for the purpose of Stockpile Stewardship. Significantly, the ability of these newly developed interatomic potentials to track additional physical variables will give new insights into the behavior of these materials under extreme conditions, where experiments are either difficult or impossible to perform. Further, the incorporation of experimental data, obtained through purpose-built experiments, will produce models of unprecedented accuracy. The active learning framework will also seek to develop potentials for carbon based systems, such as polymers and ionic liquids. Critically, these new potentials will have the ability to track additional physical variables which will make them more accurate than previous potentials and capable of capturing new physical phenomena. Due to the huge diversity in carbon based molecules, these potentials will provide new methods for rapidly simulating many possible molecular systems and accelerating the discovery of new materials for additive manufacture. Additionally, these potentials can model the behavior of conventional explosives, an area critical to Los Alamos National Laboratory missions.

Publications

Journal Articles

Fedik, N., B. T. Nebgen, N. E. Lubbers, K. M. Barros, M. Kulichenko, Y. W. Li, R. Zubatyuk, R. A. Messerly, O. Isayev and S. Tretiak. Synergy of Semiempirical Models and Machine Learning in Computational Chemistry. Submitted to *Journal of Chemical Physics*. (LA-UR-23-23011)

Gibson, T. R., S. Tretiak and S. Fernandez-Alberti. Modeling Excited State Molecular Dynamics Beyond Born-Oppenheimer Regime: Present and Future. Submitted to *Nature Computational Science*. (LA-UR-22-29704)

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Kulichenko, M., K. M. Barros, N. E. Lubbers, N. Fedik, G. Zhou, S. Tretiak, B. T. Nebgen and A. M. Niklasson. Semi-Empirical Shadow Molecular Dynamics: A PyTorch implementation. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-22-33200)

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*Li, T., Y. Wang, W. Li, D. Mao, C. J. Benmore, I. Evangelista, H. Xing, Q. Li, F. Wang, G. Sivaraman, A. Janotti, S. Law and T. Gu. Structural Phase Transitions between Layered Indium Selenide for Integrated Photonic Memory. 2022. *Advanced Materials*. **34** (26): 2108261. (LA-UR-21-30387 DOI: 10.1002/adma.202108261)

Li, W., X. Cai, N. Valdes, T. Wang, W. Shafarman, S. Wei and A. Janotti. In2Se3, In2Te3, and In2(Se,Te)3 alloys as photovoltaic materials. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-22-31892)

Li, W., Z. Wang, X. Xiao, Z. Zhang, A. Janotti, R. Sanguthevar and B. Medasani. Predicting band gaps and band-edge positions of oxide perovskites using density functional theory and machine learning. 2022. *Physical Review B*. **106** (15): 155156. (LA-UR-22-23146 DOI: 10.1103/PhysRevB.106.155156)

*Magedov, S., C. Koh, W. Malone, N. Lubbers and B. Nebgen. Bond order predictions using deep neural networks. 2021. *Journal of Applied Physics*. **129** (6): 064701. (LA-UR-21-30590 DOI: 10.1063/5.0016011)

Philip, A. M., G. Zhou and B. T. Nebgen. Computing Barrier Heights of Molecular Motors Using Deep Learning. Submitted to *Journal of Chemical Physics*. (LA-UR-22-31508)

Sifain, A. E., L. Lystrom, R. A. Messerly, J. S. Smith, B. Nebgen, K. Barros, S. Tretiak, N. Lubbers and B. J. Gifford. Predicting phosphorescence energies and inferring wavefunction localization with machine learning. 2021. *Chemical Science*. **12** (30): 10207-10217. (LA-UR-21-21632 DOI: 10.1039/D1SC02136B)

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Tretiak, S., R. Zubatyuk, M. Kulichenko, N. E. Lubbers, J. S. Smith, B. T. Nebgen, R. A. Messerly, Y. W. Li, A. I. Boldyrev, O. Isayev and N. S. Fedik. Machine Learning for Molecular Properties: Going Beyond Interatomic Potentials. Submitted to *Nature Reviews Chemistry*. (LA-UR-21-29272)

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**Peer-reviewed*

Machine Learning for Realizing Next-Generation Quantum Hardware

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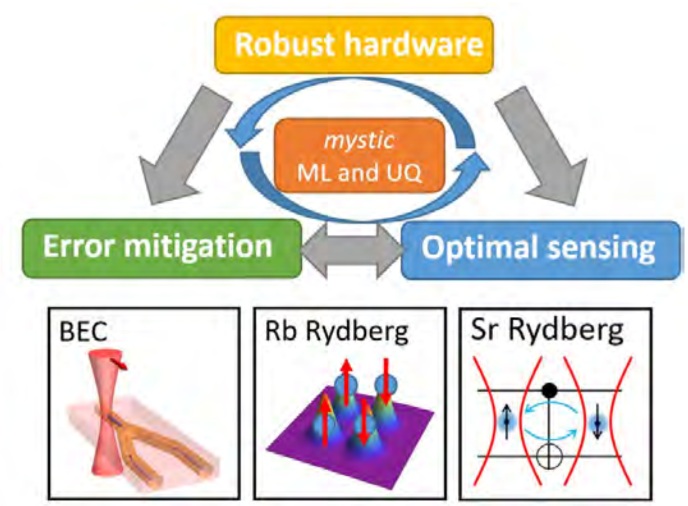
20210116DR



Our three thrusts, robust hardware, optimal sensing, and error mitigation, are supported by and interact with the machine learning (ML) backbone of this work. In particular, we base our approach around the mystic package, a framework for implementing ML and uncertainty quantification (UQ). LANL-owned hardware resources are shown at bottom. The interplay between ML and hardware enables better physics -informed ML for quantum technology, enhanced quantum sensors, and better predictive capability with near-term quantum hardware.

Project Description

Quantum technologies (QT) are today poised to revolutionize computing and sensing, with applications in fundamental science and national security. However, as quantum systems grow in size and complexity, controlling QT while preserving and optimally exploiting fragile quantum correlations becomes intractable using standard, human-directed approaches. Our ability to harness quantum effects limits the quantum advantage of a given system, be it a sensor or quantum computer. We address this challenge by integrating machine learning (ML; a powerful new set of tools for working with complex data and systems), with quantum hardware developed at Los Alamos National Laboratory to create a new generation of QT. With this approach, we discover new approaches to (1) realizing experiments with enhanced performance and robustness against environmental fluctuations, (2) generating and utilizing entangled states for optimal quantum sensing, and (3) error mitigation in quantum computing/simulation. Further, we note that this work impacts ML by incorporating physics domain knowledge into ML approaches, leveraging uncertainty quantification techniques to produce optimally robust models, and by demonstrating reproducibility in ML-based models. These are cutting-edge topics in the scientific ML community. Thus, with this synthesis of ML and QT, we advance the state of the art in ML and QT.

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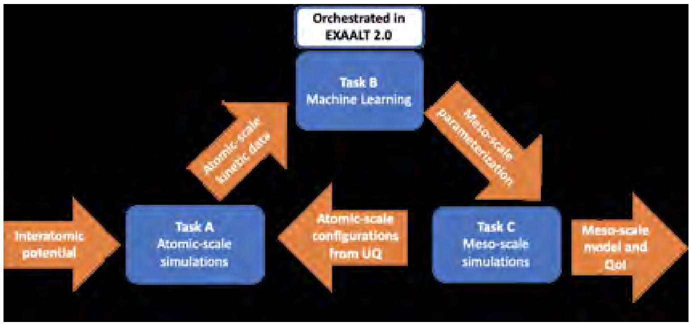
**Peer-reviewed*

Accelerated Dynamics Across Computational and Physical Scales

Danny Perez
20220063DR



Schematic of the upscaling loop that will be developed in the project. Atomistic simulations will generate large amounts of data that will be ingested by a machine learning module that will learn a model of meso-scale properties. Simulations will be carried out with this model to identify the atomistic simulations that will maximally improve the fidelity of the model's predictions. All of the simulations will execute simultaneously at scale without human intervention, maximizing the rate of information acquisition and dramatically cutting the model-development time.

Project Description

New chemically complex materials (like high entropy alloys) offer a wide range of new opportunities to optimize materials, i.e., to design safer nuclear reactors or to develop new materials with unique mechanical properties. Predicting the properties of these materials at engineering scales is however extremely challenging, and currently requires years of tedious work. Our project will harness the power of exascale computing to rigorously and automatically parameterize these engineering models from high quality simulations at the atomic scale. This capability will allow for the systematic exploration of this large materials space in search of unique candidates for applications. Our targets include nuclear materials that can tolerate high doses of radiation without affecting their properties and the deformation of materials in extreme conditions of pressure/temperature. Both these applications directly support Department of Energy's and National Nuclear Science Administration's missions and leverages the investments made in the context of the Exascale Computing Initiative.

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Reports

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*Peer-reviewed

MASS-APP: Multi-physics Adaptive Scalable Simulator for Applications in Plasma Physics

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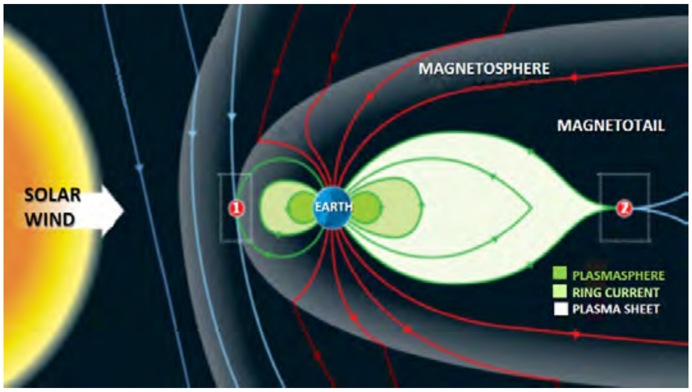

Diagram showing regions of significant distortion in the Earth's magnetic due to eruptive events on the sun. These distortions cannot be captured by current computational methodologies but will be accurately represented using our MASS-APP framework.

Project Description

Efficient and accurate coupling of the microscopic physics into the macroscopic system-scale dynamics (a.k.a. fluid-kinetic coupling) is arguably the most important and yet still unresolved problem of computational plasma physics. It impacts a wide variety of systems, including astrophysical systems (e.g. core-collapse and thermonuclear supernovae, as well as kilonovae produced in the mergers of neutron stars), the solar corona, the Earth's magnetosphere, and all the way to laboratory experiments such as those for magnetic and inertial fusion energy. Due the enormous range of dynamically relevant scales characterizing such problems, direct calculations, which solve the whole spectrum of scales, are not going to be possible for the foreseeable future. While there have been numerous attempts to bridge the large and small scale physics, a flexible, multi-scale framework for plasma physics applications valid across multiple regimes has so far remained elusive. Multi-physics Adaptive Scalable Simulator (MASS-APP) will be the first adaptive, multi-scale, multi-physics exascale-ready computational framework capable of accurately solving system-scale (macroscopic) plasma physics problems including small-scale (microscopic) physics. It will provide accurate answers to previously unsolved problems in a multitude of fields, from extreme space weather events of interest to global security, to astrophysics, and to Los Alamos National Laboratory-centric applications like inertial confinement fusion.

Publications

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Brady, P. T. and D. Livescu. High-Order Cut-Cell Methods for High-Fidelity Flow Simulations. Presented at *International Conference on Computational Fluid Dynamics*, Maui, Hawaii, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26667)

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Delzanno, G. L. Systems science of codes. Presented at *GEM Summer Workshop*, honolulu, Hawaii, United States, 2022-06-19 - 2022-06-26. (LA-UR-22-25767)

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Koshkarov, O., G. L. Delzanno, V. Roytershteyn and C. Pagliantini. Enabling Optimizations for Global Magnetospheric Kinetic Simulations with Reduced Kinetic Spectral Models. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-17. (LA-UR-22-30526)

**Peer-reviewed*

Quantum Chemistry using Quantum Computers

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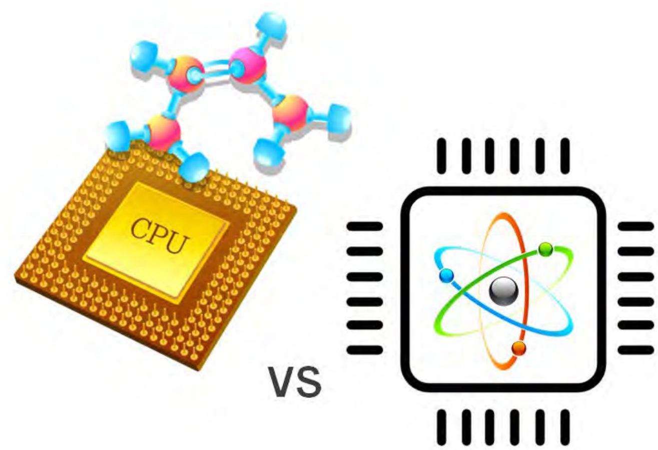
20200056DR



Simulation of molecules and materials, due to their quantum nature, is expected to be one of the first immediate applications of near-term quantum computers directly impacting LANL present and future missions. The project develops new hybrid classical-quantum algorithms to solve quantum chemistry problems on noisy intermediate-scale quantum (NISQ) devices.

Project Description

Quantum computers (QC) promise to be a game changer for materials science modeling, an appropriate implementation, but the tools are yet to be developed. Hybrid quantum-classical algorithms are the current state-of-the-art in the noisy intermediate-state quantum (NISQ) era. Existing advances such as variational quantum eigensolver (VQE) solvers need quality initial states (ansatzes) and minimal number of qubits for each problem at hand (currently limited to very small molecules only). Subsequently, casting the original problems in terms of novel Information Science and Technology (IS&T) algorithms and software layers is a key ingredient for solving the quantum problem and demonstrating practical utility of existing QC hardware. Our particular innovation is the development of algorithms able to achieve the qubit size reduction for quantum solver methods based on Machine Learning, Quantum Graph Partitioning, High-Performance Computing (HPC) and Quantum Computing unique to Los Alamos National Laboratory and without sacrificing accuracy. This project is delineated into three distinct tasks: 1) develop strategies and algorithms to perform static quantum chemistry calculations on medium-to-large size molecules on QCs; 2) develop quantum molecular dynamics on QCs; 3) extend algorithms to excited states and non-equilibrium molecular dynamics beyond the Born-Oppenheimer approximation.

Technical Outcomes

The state-of-the-art quantum chemistry algorithms developed by this project are general and provide a novel set of capabilities in quantum computing relevant for treating materials science and other problems that are of direct applicability to Los Alamos National Laboratory, Department of Energy (DOE), and National Nuclear Security Administration (NNSA) missions. All of these novel algorithms represent a significant advance in quantum computing capabilities.

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Posters

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**Peer-reviewed*

Prioritizing the Prior: Advanced Inversion Algorithms for Scientific Data Analysis

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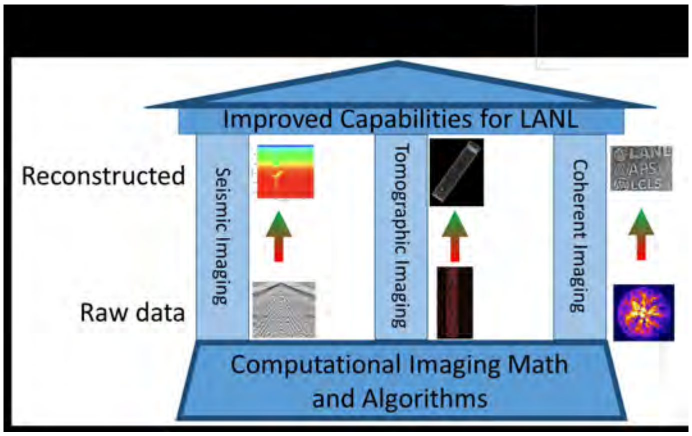

Solving inverse problems is common to a wide range of applications ranging from seismic imaging, to tomography, to coherent imaging/ptychography. This LDRD funded effort brings together experts for these techniques with experts in solving inverse problems to develop a common highly efficient analysis framework and enable access to novel approaches such as machine learning to all fields.

Project Description

There is a diverse range of mission-critical problems both at the Laboratory and within the Department of Energy (DOE) that involve challenging inverse problems with common properties. The full value of the knowledge that can be gained from the experiments depends critically on the effectiveness of the solutions to these inverse problems, which are often very challenging to solve. While there is a wealth of domain expertise at the Laboratory, we have a much more limited capability in the development of the required mathematics and algorithms for solving difficult inverse problems. We propose to establish such a capability, motivated by the recognition that many of the problems that are entirely unrelated from a physics perspective, share significant common properties at the level of the mathematics of inverse problems. This project will develop effective solution-space models that are essential to obtaining reliable solutions of the numerous problems encountered within Laboratory mission areas such as stockpile stewardship, materials science, and energy security. All of these application domains involve very difficult inverse problems for which substantial improvements are expected to be possible, and in some cases, for which there are no current solutions.

Technical Outcomes

The project was successful in achieving the main technical goals. New algorithms were developed to address the need for advanced regularization of medium scale imaging problems, as well as the need for calibration of the mathematical model of the imaging process. Significant practical contributions were made to imaging needs in all four application focus areas of neutron imaging, dynamic tomography, coherent imaging, and seismic imaging.

Publications

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**Peer-reviewed*

In-Situ Inference: Bringing Advanced Data Science into Exascale Simulations

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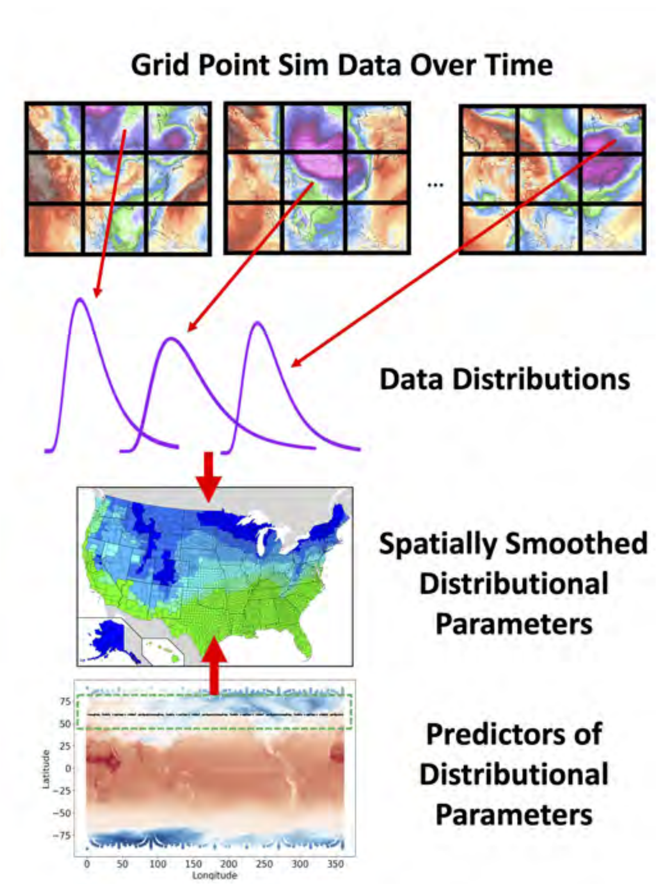

Exascale simulations will produce more data that can saved for later analysis. The project team is developing methods to analyze this data as the simulation runs, with Bayesian hierarchical models. The methods are implemented on parallel computing architectures for distributed, streaming data. Here the team will model climate extremes of polar vortex events to understand possible connections with high latitude winds. Data at each simulation grid point are modeled with extreme value distributions. The parameters of these distributions are similar across neighboring grid points and functionally connected with wind speeds at high latitudes. This enables to team to learn important spatial structure and causal relationships.

Project Description

Predictive simulations on large-scale supercomputers are at the heart of computational science in a range of mission areas spanning energy, nuclear stockpile stewardship, and physical and biological science and engineering. Modern high performance computing architectures now generate far more scientific data than can be saved to disk for later analysis, leading to a potential crisis in our ability to understand and use the predictions of scientific models. This requires moving the analysis into the simulation itself, “in-situ”. Advanced statistical analysis, or “inference”, methods are currently not designed to scale to in-situ deployment within Department of Energy exascale supercomputers. We will develop new parallel statistical algorithms capable of analyzing vast quantities of spatial and time varying data as they are being generated by physics simulations. This will enable an unprecedented level of detail in our ability to analyze the highly complex phenomena that exascale models will simulate, such as the risk and causes of rare, high-impact events such as winter storms or solar-geomagnetic space hazards.

Technical Outcomes

The project was successful. The project focused on in-situ methods for modeling spatial simulation data. The team developed two new spatial model formulations for in-situ modeling; a fast neural network-based approach to fitting spatial models; and a new implementation of principal components analysis. Additionally, the team developed in-situ methods for regression models for continuous, binary, count, and extreme value data. These served as building blocks to solve problems in climate and space weather.

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*Peer-reviewed

Scale-bridging Hydrodynamic Simulations

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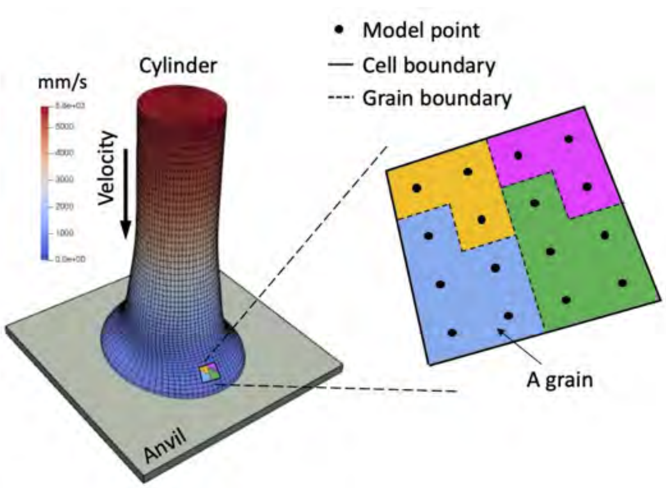

A new spatial and temporal scale-bridging hydrodynamic approach is being developed at LANL to capture mesoscale physics in full-scale simulations of solid dynamics in engineering and physics applications. The new approach evolves mesoscale physics models on a fine grid of points within a macroscale cell — combined with a strong two-way coupling across scales — to replace a finely resolved mesh for efficient, high-fidelity simulations.

Project Description

The microstructure of a solid varies depending on the composition and manufacturing processes. Differences in the microstructure can lead to significant differences in the macroscale (i.e., bulk) dynamic behavior of the solid across physical regimes. In explosively driven flyer plate experiments, variations in the microstructure can significantly alter the solid dynamics over the time scale of millionths of a second. In inertial confinement fusion (ICF) experiments, the microstructure of a solid can create perturbations on the solid-gas surface on the time scale of billionths of a second that grow and reduce the nuclear fusion yields. The proposed research is to create a novel simulation approach to capture mesoscale physics (i.e., the physics at the microstructure level) in macroscale hydrodynamic simulations. The proposed work seeks to close an existing algorithmic gap with bridging between mesoscale physics and macroscale hydrodynamic simulations. The new scale-bridging approach will significantly improve the physical fidelity of full-scale engineering and physics simulations of solids with high internal microstructural variation, such as additively manufactured (AM) metals, complex multiphase alloys, foams, metals, and composite materials.

Technical Outcomes

This project successfully researched a novel high-fidelity scale-bridging approach to simulate material dynamics that is also ideal for acceleration on graphics processing unit (GPU)-based computer architectures for timely simulations. The approach tightly couples a Lagrangian linear finite element hydrodynamic method with a new multi-scale elasto-viscoplastic material model. The software was written to run on central processing unit (CPUs)+GPUs and delivers exceptional run times.

Publications

Presentation Slides

Heilman, E. and C. Roth. Modeling the Dynamics of Solids on CPUs and GPUs. . (LA-UR-22-27651)

Yenusah, C. O., T. W. Stone, N. R. Morgan, R. W. Robey, Y. Liu and L. Chen. INCORPORATING PERFORMANCE PORTABILITY AND DATA-ORIENTED DESIGN IN PHASE-FIELD MODELING. Presented at *nternational Design Engineering Technical Conferences and Computers and Information in Engineering Conference*, St. Louis, Missouri, United States, 2022-08-14 - 2022-08-17. (LA-UR-22-25455)

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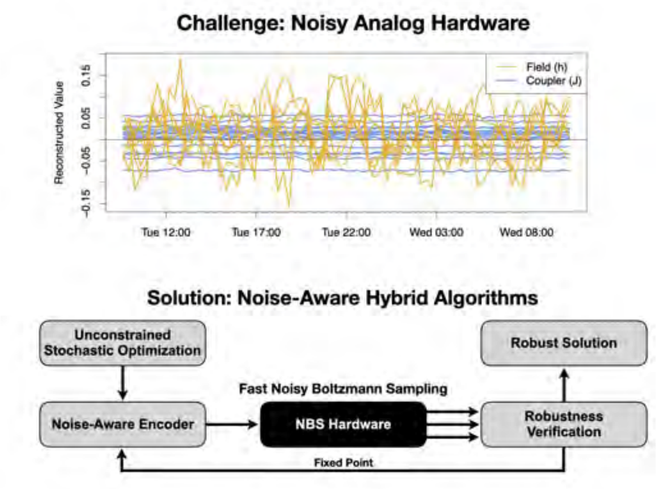
**Peer-reviewed*

Accelerating Combinatorial Optimization with Noisy Analog Hardware

Carleton Coffrin
20210114ER



The slowing advance of traditional digital computing hardware has spurred a renaissance in analog computing platforms, which are dedicated to performing specialized computational tasks. In such platforms, analog noise presents a fundamental challenge to conducting computations (top). This work proposes to leverage analog noise as a strength, which can be harnessed to design high-performance hybrid algorithms for stochastic optimization (bottom). The objective of this work is to establish that analog-accelerated stochastic optimization algorithms can significantly outperform all known alternatives.

Project Description

The slowing advance of traditional digital computing hardware has spurred a renaissance in analog computing platforms, which are dedicated to performing specialized computational tasks. This work will help Los Alamos National Laboratory (LANL) scientists develop a deeper understanding of what computational benefits these analog computing platforms can provide. This understanding is a critical first step to integrating analog computing platforms into mission critical computational tasks conducted at LANL for the Department of Energy/ National Nuclear Security Administration.

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Conference Papers

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Presentation Slides

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Coffrin, C. J. Quantum Simulation with Quantum Annealing Computers. . (LA-UR-22-23961)

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Coffrin, C. J. Physics Informed ML for Quantum Computers. . (LA-UR-22-28979)

Coffrin, C. J. Quantum Computing and AI. . (LA-UR-22-29557)

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**Peer-reviewed*

Strategies for Topological Quantum Computing with Braiding of Vortices and Skyrmions

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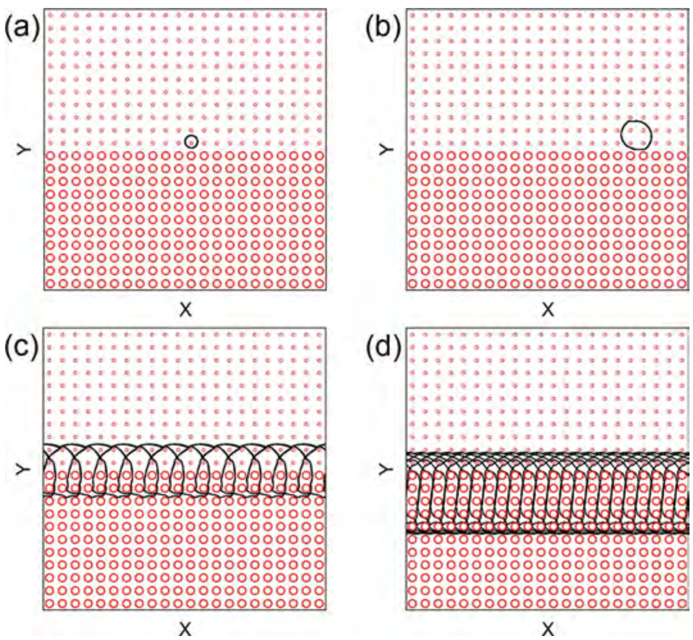

The goal of this project is to create quantum logic gates by entangling Majorana fermions. This requires having the ability to cause vortices or skyrmions to encircle sets of pinning sites dynamically, as shown in panel (b) where a single skyrmion encircles four skyrmions. The other ingredient is to be able to translate the particle performing the encircling, as illustrated in panels (c) and (d). The team identified a geometry which can achieve both of these effects by using an interface between large and small pinning sites, as shown in panel (a). Published in J. Mag. Mag. Mater. 528, 167710 (2021).

Project Description

Quantum computing utilizes the properties of quantum mechanics to perform certain computations much more rapidly than a classical computer and to solve problems that are entirely beyond their reach. Realizing quantum computing will have enormous implications for national security, economic, and scientific advances. Department of Energy (DOE) and Los Alamos National Laboratory (LANL) have identified quantum computing as an area of concentration. Topological quantum computers (TQC) bypass the problem of short qubit decoherence times and logical errors by harnessing topologically protected qubits made from quasiparticles such as Majorana Fermions (MFs), but robust methods for manipulating the MFs to form quantum logic gates are still lacking. This project uses superconducting vortices and magnetic skyrmions that are stabilized by a periodic pinning array and manipulated with scanning tips or bulk currents to realize the logic operations needed for a physical realization of a TQC. We will identify the most efficient logic gate designs based on our novel concept and will work with external experimental groups who can test and verify the logic gate operations. If successful, this work will pave the way towards the construction of the first practical, scalable TQC device, placing LANL at the forefront of quantum computing.

Publications

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Posters

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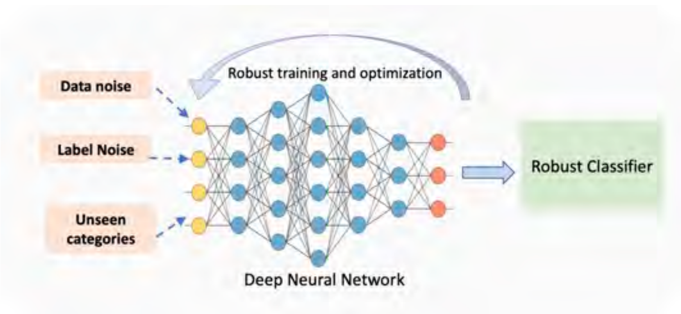
**Peer-reviewed*

Deep Learning in a Noisy World: Algorithms for Robust Training and Predictive Uncertainty

Sunil Thulasidasan
20210356ER



State-of-the-art Deep Neural Networks (DNNs) need to be trained on large amounts of clean, well-labeled data -- which is an infeasible requirement -- and are often unable to provide reliable estimates of predictive uncertainty. This effort tackles both of these issues in various ways: by keeping track of how the classifier learns during training, by incorporating novel loss functions for training and also by using novel data augmentation techniques. These methods not only result in being able to learn robustly in the presence of corrupted data, but also result in better estimates of predictive uncertainty.

Project Description

Machine learning using deep neural networks – also called "Deep Learning" (DL) - has been at the center of practically every major advance in artificial intelligence over the last several years and there is now tremendous interest in using DL-based systems in all domains where computers can be used to make predictions after being trained on large quantities of data. The proposed work will develop algorithms to overcome two significant challenges when using DL for mission applications. 1. State-of-the-art Deep Neural Networks (DNNs) -- that form the core of the deep learning pipeline -- need to be trained on large amounts of clean, well-labeled data, which is often infeasible in the real world where noisy data is the norm. 2. Trained DNNs are unable to provide reliable estimates of predictive uncertainty, a crucial need in mission space. Standard training techniques result in over-confident predictions, especially when presented with data from categories not seen during training. That is, standard deep models "do not know what they don't know". The proposed effort will build on recent fundamental advances by our team in these areas to develop a broadly applicable, general-purpose framework for improving robustness and predictive uncertainty in deep learning.

Publications

Journal Articles

Porter, R. B., B. G. Zimmer, Q. Nguyen and V. Jatla. End-to-End Learning of Hierarchical Watersheds. Submitted to *Journal of Mathematical Imaging and Vision*. (LA-UR-21-20143)

Conference Papers

Singh, H. S. Synthetic-to-Real Domain Adaptation for Autonomous Driving. Presented at *Smoky Mountains Challenge*. (Oak Ridge, Tennessee, United States, 2021-10-18 - 2021-10-18). (LA-UR-21-30388)

Thulasidasan, S., S. Thapa, S. Dhaubhadel, G. Chennupati, T. Bhattacharya and J. Bilmes. An Effective Baseline for Robustness to Distributional Shift. Presented at *20th IEEE INTERNATIONAL CONFERENCE ON MACHINE LEARNING AND APPLICATIONS*. (Pasadena, California, United States, 2021-12-13 - 2021-12-16). (LA-UR-21-30506)

Reports

Pang, X., S. Thulasidasan and L. J. Rybarcyk. Autonomous Control of a Particle Accelerator using Deep Reinforcement Learning. Unpublished report. (LA-UR-20-28238)

Singh, H. S. and S. Thulasidasan. Domain Adaptation using Neural Style Transfer. Unpublished report. (LA-UR-22-30641)

Thulasidasan, S., A. A. Jivan, T. Bhattacharya, G. Chennupati and J. Bilmes. A Control-Theoretic Approach to Robust Learning in the Presence of Label Noise. Unpublished report. (LA-UR-21-30505)

Posters

Singh, H. S. Synthetic-to-Real Domain Adaptation for Autonomous Driving. Presented at *SMC Data Challenge 2021*, Oak Ridge, Tennessee, United States, 2021-10-18 - 2021-10-18. (LA-UR-21-30163)

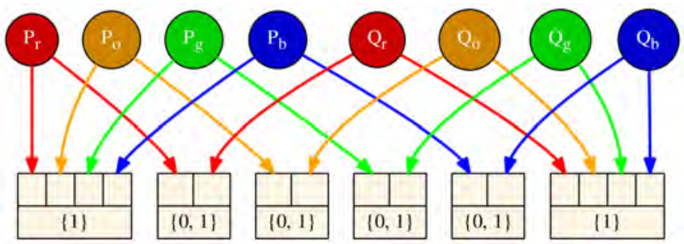
**Peer-reviewed*

Information Science and Technology

Exploratory Research
Continuing Project

Unifying Circuit-Model Quantum Computing and Quantum Annealing

Scott Pakin
20210397ER



Excerpt of a map-coloring problem expressed in NchooseK. NchooseK is a new programming model being developed by this LDRD project. The example shows how to express that two adjacent regions on a map, P and Q, must each have exactly one color ("{1}") and that either zero or one of P and Q can be red, can be orange, etc. ("{0, 1}"); they cannot both have the same color. NchooseK will satisfy these constraints on a classical computer, a quantum annealer, or a circuit-model quantum computer, making it the first high-level program model to target such radically different computational models.

Project Description

In the stockpile-stewardship arena, national security is largely dependent on who can out-compute whom. This is why all the National Nuclear Security Administration (NNSA) laboratories and other government national-security groups have traditionally invested so heavily in state-of-the-art supercomputers. It is also why quantum computing is now so appealing. For certain problems, it is believed that a single quantum computer will one day outperform all of the world's conventional computers combined. Alas, quantum programming not only exhibits virtually no traits in common with classical programming but is extremely challenging. Forthcoming quantum hardware with large computational abilities offers little benefit if only a small number of quantum-computing experts are able to program such devices. This project addresses the programmability problem by attempting to define and implement a new programming model that is relatively easy for non-experts in quantum computing to learn and that can be implemented—with varying performance characteristics—on different types of quantum (and classical) computers with little or no modification to programs. If successful, when high-performance quantum computers are finally available, programmers and computational scientists in national-security areas will be able to take advantage of them.

Publications

Conference Papers

Pakin, S. D. A Simple Heuristic for Expressing a Truth Table as a Quadratic Pseudo-Boolean Function. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Online, New Mexico, United States, 2021-10-18 - 2021-10-22). (LA-UR-21-25343)

Wilson, E. J., F. Mueller and S. D. Pakin. Combining Hard and Soft Constraints in Quantum Constraint-Satisfaction Systems. Presented at *Supercomputing - The International Conference for High Performance Computing, Networking, Storage and Analysis*. (Dallas, Texas, United States, 2022-11-13 - 2022-11-18). (LA-UR-22-23117)

Wilson, E., F. Mueller and S. D. Pakin. Mapping Constraint Problems onto Quantum Gate and Annealing Devices. Presented at *2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS)*. (St. Louis, Missouri, United States, 2021-11-15 - 2021-11-15). (LA-UR-21-30718)

Reports

Pakin, S. D. Progress Report: q20_pakin. Unpublished report. (LA-UR-22-24554)

Pakin, S. D. Annual Report: w21_nchoosek. Unpublished report. (LA-UR-22-24858)

Pakin, S. D. Preparing Equal Superpositions of n Basis States. Unpublished report. (LA-UR-22-28998)

Presentation Slides

Pakin, S. D. Running Classical Programs on a Quantum Annealer. . (LA-UR-21-23768)

Pakin, S. D. A Simple Heuristic for Expressing a Truth Table as a Quadratic Pseudo-Boolean Function. Presented at *IEEE International Conference on Quantum Computing and Engineering (QCE 21)*, Online, New Mexico, United States, 2021-10-17 - 2021-10-22. (LA-UR-21-29644)

Pakin, S. D. Running a Quantum Annealer in an HPC Data Center. Presented at *First International Workshop on Integrating High-Performance Computing with Quantum Computing (WIHPQC)*, Online, New Mexico, United States, 2021-10-20 - 2021-10-20. (LA-UR-21-29917)

Pakin, S. D. Project Appraisal: Unifying Circuit-Model Quantum Computing and Quantum Annealing (20210397ER). . (LA-UR-21-31655)

Pakin, S. D. Bringing Quantum Computing the the Masses. Presented at *Tri-lab ASC Quantum Computing meeting*, Albuquerque, New Mexico, United States, 2022-04-19 - 2022-04-20. (LA-UR-22-23222)

Pakin, S. D. q20_pakin: Quantifying Quantum Processor Fidelity. . (LA-UR-22-24528)

Pakin, S. D. w21_nchoosek: Precomputing Quadratic Pseudo-Boolean Functions. . (LA-UR-22-24857)

Pakin, S. D. Quantum Programming Made Easy. Presented at *Scientific Applications of Quantum Annealers*, Telluride, Colorado, United States, 2022-06-11 - 2022-06-15. (LA-UR-22-25478)

Pakin, S. D. Quantum Computers in High-Performance Computing Centers. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Broomfield, Colorado, United States, 2022-09-18 - 2022-09-23. (LA-UR-22-29653)

Pakin, S. D. QC and HPC: Together Again at Last\xe2\x80\xa6for the Very First Time. Presented at *Workshop on Integrating High-Performance Computing with Quantum Computing*, Broomfield, Colorado, United States, 2022-09-21 - 2022-09-21. (LA-UR-22-29744)

Pakin, S. D. and E. G. Rieffel. Introduction to Quantum Computing: Proposal for a full-day SC22 tutorial. Presented at *Supercomputing - The International Conference for High Performance Computing, Networking, Storage and Analysis*, Dallas, Texas, United States, 2022-11-13 - 2022-11-18. (LA-UR-22-23614)

Wilson, E., F. Mueller and S. D. Pakin. Mapping Constraint Problems onto Quantum Gate and Annealing Devices. Presented at *Second International Workshop on Quantum Computing Software*, St. Louis, Missouri, United States, 2021-11-15 - 2021-11-15. (LA-UR-21-30483)

Wilson, E., F. Mueller and S. D. Pakin. Combining Hard and Soft Constraints in Quantum Constraint-Satisfaction Systems. Presented at *Supercomputing - The International Conference for High Performance Computing, Networking, Storage and Analysis*, Dallas, Texas, United States, 2022-11-13 - 2022-11-18. (LA-UR-22-31731)

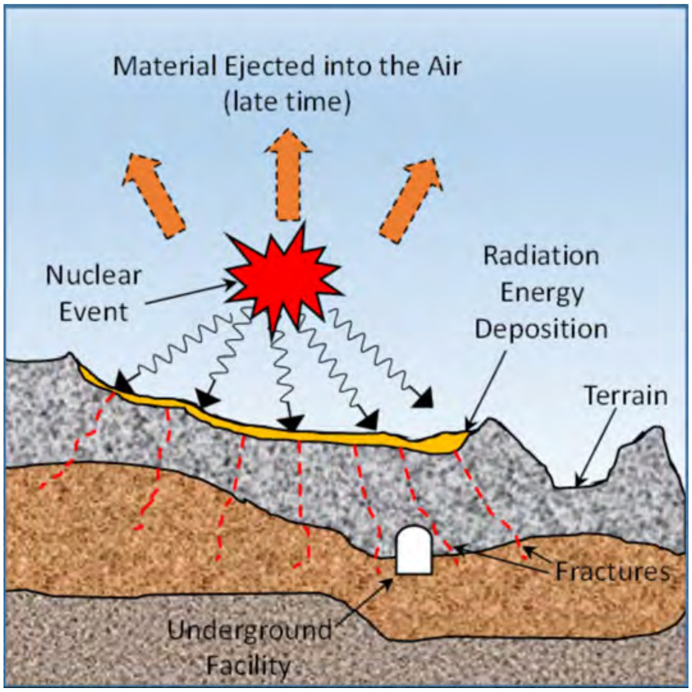
Posters

Wilson, E. J., F. Mueller and S. D. Pakin. NchooseK: Constraint Based Quantum Computing. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22086)

**Peer-reviewed*

Resolving the Energy Transfer from a Nuclear Energy Source to the Ground

Esteban Rougier
20210436ER



How much energy is transferred to the ground after an aerial nuclear detonation? The answer to this question contains a big margin of uncertainty. The main purpose of this research is to reduce this uncertainty and provide a better constraint description of how much energy is actually coupled into the ground. This will be achieved by accounting for the contribution of the radiation energy via the incorporation of radiation transport solvers into the existing Hybrid Optimization Software Suite (HOSS)-Fluid-Solid Interaction Solver (FSIS) framework. Once completed, this coupled solver will allow for improved nuclear weapons effects estimates, i.e., crater dimensions, amount of material ejected into the air, etc.

Project Description

The main objective of this theoretical and computational project is to obtain a better understanding of the energy transfer mechanisms between a nuclear weapon surface burst and the surrounding solid media. The expected result is to reach an uncertainty reduction for cratering and lofted volume (ground and nearby materials being lifted into the atmosphere) estimates, thereby improving confidence on how much material would be available for radioactive fallout to occur for a particular nuclear event. A correlated result is to improve the fidelity of simulated nuclear weapons effects on both above ground and underground structures and facilities. Regarding the impact on Department of Energy/National Nuclear Security Administration missions, it has been recognized that to be able to predict the effects of a nuclear weapon detonation in a local and regional context is critical to planning for and responding to a nuclear detonation. Recent computer advances and computational techniques now allow us to tackle these challenges that we were previously unable to address. This effort sets a cornerstone in our pathway to improve the fidelity of nuclear weapon effects estimates in a variety of important scenarios.

Publications

Journal Articles

Lei, Z., A. Munjiza, E. Rougier, E. E. Knight and C. R. Bradley. AXISYMMETRIC FDEM FORMULATION FOR LARGE DEFORMATION SOLIDS. Submitted to *International Journal for Numerical Methods in Engineering*. (LA-UR-22-30243)

Lei, Z., A. Munjiza, E. Rougier, E. E. Knight and C. R. Bradley. AXISYMMETRIC FDEM FORMULATION FOR LARGE DEFORMATION SOLIDS. Submitted to *International Journal for Numerical Methods in Engineering*. (LA-UR-22-30924)

*Lei, Z., E. Rougier, E. E. Knight, M. Zang and A. Munjiza. Impact Fracture and Fragmentation of Glass via the 3D Combined Finite-Discrete Element Method. 2021. *Applied Sciences*. **11** (6): 2484. (LA-UR-21-21493 DOI: 10.3390/app11062484)

Rougier, E. and A. Hunter. Fracture Mechanics—Theory, Modeling and Applications. 2021. *Applied Sciences*. **11** (16): 7371. (LA-UR-21-27423 DOI: 10.3390/app11167371)

Reports

Rougier, E. and A. M. Padilla. YEARLY REPORT FOR THE PERIOD Jan-Dec 2021 - IC Project: w20_earthquake. Unpublished report. (LA-UR-22-24537)

Till, A. T. Discretization Writeup for Grey Flux-Limited Radiation Diffusion. Unpublished report. (LA-UR-20-29323)

Presentation Slides

Knight, E. E., Z. Lei, B. J. Euser, S. H. S. Boyce, A. Munjiza and E. Rougier. HOSS OVERVIEW. . (LA-UR-21-29085)

Lei, Z., E. E. Knight, E. Rougier, B. J. Euser, S. H. S. Boyce and A. Munjiza. Enhanced Contact and Fracture Solutions for FDEM. Presented at *WCCM-ECCOMAS 2020*, Barcelona, Spain, 2021-01-11 - 2021-01-15. (LA-UR-20-30016)

Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. The Combined Finite-Discrete Element Method (FDEM): An Overview. . (LA-UR-21-29098)

Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. The Combined Finite-Discrete Element Method (FDEM): An Overview. . (LA-UR-21-29089)

Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. Algorithm Aspects of the Combined Finite-Discrete Element Method: An Overview. Presented at *Workshop "FDEM-2022 - Modeling innovations and numerical experiments in geomechanics"*, Toronto, Canada, 2022-12-09 - 2022-12-09. (LA-UR-22-32693)

Okubo, K., C. Villafuerte, E. Rougier and H. S. Bhat. Dynamic earthquake ruptures and its radiations with off-fault fracture network in various spatial resolutions. Presented at *Japan Geoscience Union Meeting*, Chiba, Japan, 2023-05-21 - 2023-05-21. (LA-UR-23-21603)

Rougier, E., E. E. Knight, Z. Lei, B. J. Euser, S. H. S. Boyce and A. Munjiza. LANL HOSS Modeling Capabilities. . (LA-UR-21-29065)

Rougier, E., E. E. Knight, Z. Lei and A. Munjiza. HOSS Development and Applications A Historical Perspective. Presented at *FDEM Workshop*, Toronto, Canada, 2022-12-09 - 2022-12-09. (LA-UR-22-32718)

Rougier, E., Z. Lei, B. J. Euser, A. Munjiza and E. E. Knight. Fluid-Solid Interaction via the Combined Finite-Discrete Element Method. . (LA-UR-21-24172)

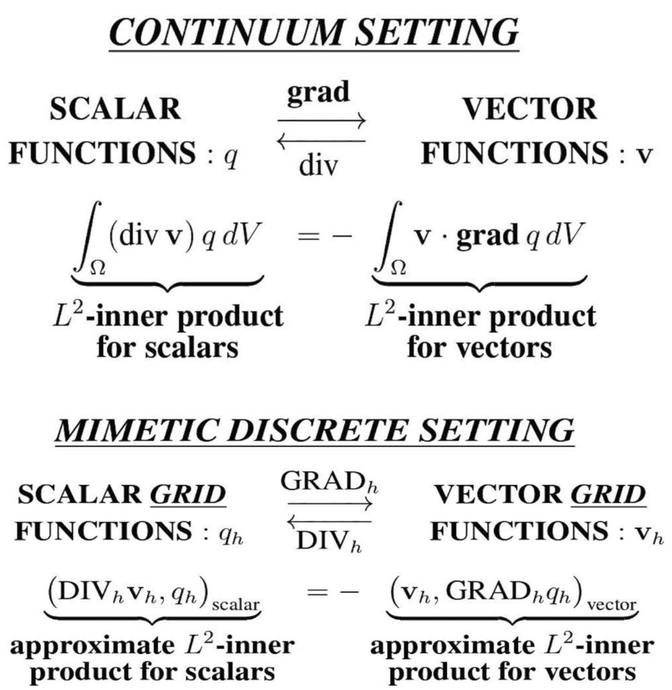
Rougier, E., Z. Lei, B. J. Euser, E. E. Knight and A. Munjiza. Fluid-Structure Interaction Problems via the Combined Finite-Discrete Element Method. Presented at *14th World COngress on Computational Mechanics*, Paris, France, 2021-01-11 - 2021-01-11. (LA-UR-20-29727)

Rougier, E. and A. M. Padilla. YEARLY REPORT FOR THE PERIOD Jan-Dec 2021 - IC Project: w20_earthquake. . (LA-UR-22-24516)

**Peer-reviewed*

Mimetic Tensor-Train Algorithms for High-Dimensional Partial Differential Equations (PDEs) without the Curse of Dimensionality

Gianmarco Manzini
20210485ER



Mimetic divergence and gradient operators apply to vector and scalar grid functions and satisfy exactly a discrete duality relation (right) as their counterparts in the continuum setting (left). The TT-format that is used in the project offers a practical way to build such discrete operators in any number of dimensions.

Project Description

This project will focus on two very specific goals: (i) developing numerical methods for solving high-dimensional partial differential equations (PDEs), and (ii) developing numerical methods for solving PDEs with a high number of degrees of freedom. This is a basic research project with immense potential impact; this project's results can potentially be a "game changer" in the compute treatment in a variety of fields and applications, including national engineering problems that require massive numerical simulations.

Publications

Journal Articles

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Submitted to *Numerical Linear Algebra with Applications*. (LA-UR-21-26100)

Manzini, G., P. M. D. Truong, R. Vuchov and B. Alexandrov. The tensor-train mimetic finite difference method for three-dimensional Maxwell's wave propagation equations. 2023. *Mathematics and Computers in Simulation*. (LA-UR-22-28983 DOI: 10.1016/j.matcom.2023.03.026)

Conference Papers

Manzini, G., B. Alexandrov, P. M. D. Truong and R. Vuchkov. The tensor-train mimetic finite difference method for three-dimensional Maxwell's wave propagation equations. Presented at *Large-Scale Scientific Computations*. (Sozopol, Bulgaria, 2023-06-05 - 2023-06-09). (LA-UR-23-21109)

Manzini, G., E. W. Skau, P. M. D. Truong and R. Vangara. Nonnegative tensor-train low-rank approximations of the Smoluchowski equation. Presented at *13th International Conference on "Large-Scale Scientific Computations"*. (Sozopol, Bulgaria, 2021-06-07 - 2021-06-11). (LA-UR-21-23325)

Manzini, G. and M. Martinelli. A Functional Tensor Train Library in RUST for Numerical Integration and Resolution of Partial Differential Equations. Presented at *LSSC-23*. (Sozopol, Bulgaria, 2023-06-05 - 2023-06-09). (LA-UR-23-22254)

Vuchkov, R., B. Alexandrov, G. Manzini, E. W. Skau and P. M. D. Truong. Tensor-Train-Based Composite Algorithms For High-Dimensional Numerical Integration. Presented at *Large-Scale Scientific Computations*. (Sozopol, Bulgaria, 2023-06-05 - 2023-06-09). (LA-UR-23-21108)

Reports

Alexandrov, B., G. Manzini, E. W. Skau, P. M. D. Truong and R. Vuchov. Challenging the curse of dimensionality in multidimensional numerical integration by using a low-rank tensor-train format. Unpublished report. (LA-UR-22-29661)

Alexandrov, B., G. Manzini, E. W. Skau and P. M. D. Truong. Composite numerical integration on the multidimensional hypercube using low-rank tensor-train cross representation. Unpublished report. (LA-UR-21-24664)

Manzini, G., B. Alexandrov, K. O. Rasmussen and P. M. D. Truong. White paper - Ultra-fast Tensor Solvers for Ultra-big PDEs. Unpublished report. (LA-UR-21-30691)

Presentation Slides

Alexandrov, B., G. Manzini, E. W. Skau, P. M. D. Truong and R. Vuchkov. Tensor Train Network and its Applications to Numerical Integration and Partial Differential Equations. Presented at *Optimization Seminar, University of California, Merced*, Merced, California, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-29268)

Manzini, G. A non-negative tensor-train based method for the Smoluchowski coagulation equation.. Presented at *13th International Conference on Large-Scale Scientific Computations*, Sozopol, Bulgaria, 2021-06-07 - 2021-06-11. (LA-UR-21-25537)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *16th U.S. National Congress on Computational Mechanics (USNCCM-16)*, Chicago, Illinois, United States, 2021-07-25 - 2021-07-29. (LA-UR-21-25539)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *SIAM Conference on Mathematical & Computational Issues in the Geosciences (GS21)*, Milano, Italy, 2021-06-21 - 2021-06-24. (LA-UR-21-25538)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *16th U.S. National Congress on Computational Mechanics (USNCCM-16) - LA-UR-21-25539*, Chicago, Illinois, United States, 2021-07-25 - 2021-07-29. (LA-UR-21-25671)

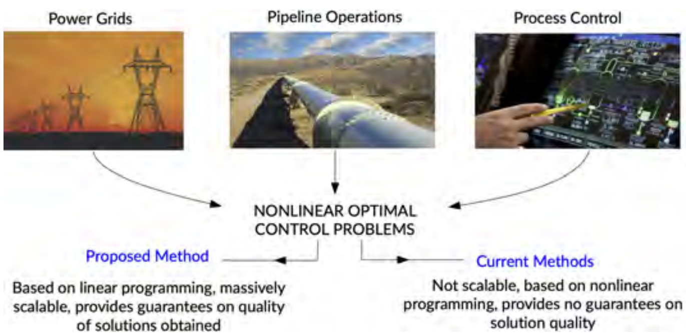
Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *SIAM Conference on Mathematical & Computational Issues in the Geosciences (GS21)*, Milano, Italy, 2021-06-21 - 2021-06-24. (LA-UR-21-25672)

Manzini, G., E. W. Skau and P. M. D. Truong. Mimetic Tensor-Train Algorithms for High-Dimensional PDEs. . (LA-UR-22-31460)

**Peer-reviewed*

Fast, Linear Programming-Based Algorithms with Solution Quality Guarantees for Nonlinear Optimal Control Problems

Kaarthik Sundar
20220006ER



In many mission-critical applications such as operation of pipeline infrastructure networks, formation control of CubeSat, disease spread management, etc. it is of interest to drive a nonlinear dynamical system from an initial state to a desirable final state while optimizing a performance index. Such problems are referred to as Nonlinear Optimal Control Problems. Current algorithmic approaches, based on nonlinear programming techniques, have scalability issues and do not provide any guarantees on the solution they provide. This project aims to develop a massively scalable approach based on linear programming to compute solutions to these problems with a guarantee on solution quality.

Project Description

Analysis and efficient operation of critical pipeline infrastructure (natural gas, water, etc.) is a crucial national security challenge; all the more so given recent impacts to natural gas pipelines by severe winter weather events. The socio-economic systems of the United States depend on the reliable delivery of energy, water, etc. in order to function normally. As a result, Department of Energy and other stakeholders are tasked with ensuring these systems are operated efficiently in a safe and robust manner. However, the ability of policy makers to analyze and protect these systems is limited by the computational requirements of solving related problems in these systems at a nation-wide scale. This project is focused squarely on building the fundamental algorithms that reduce these computational burdens and facilitate the ability of policy makers to make informed decisions on how to best secure the nation's critical pipeline infrastructure.

Publications

Journal Articles

Kazi, S. R., K. Sundar, S. Srinivasan and A. V. Zlotnik. Modeling and Optimization of Steady Flow of Natural Gas and Hydrogen Mixtures in Pipeline Networks. Submitted to *IEEE Transactions on Control of Network Systems*. (LA-UR-22-32518)

Srinivasan, S., K. Sundar, V. Gyrya and A. V. Zlotnik. Numerical Solution of the Steady-State Network Flow Equations for a Non-Ideal Gas. Submitted to *IEEE Transactions on Control of Network Systems*. (LA-UR-22-21789)

Srinivasan, S. and N. Panda. A unified treatment of matrix calculus on structured spaces. Submitted to *Indian Journal of Pure and Applied Mathematics*. (LA-UR-23-23471)

Tasseff, B. A., R. W. Bent, C. J. Coffrin, C. Barrows, D. Sigler, J. Stickel, A. S. Zamzam, Y. Liu and P. Van Hentenryck. Polyhedral Relaxations for Optimal Pump Scheduling of Potable Water Distribution Networks. Submitted to *INFORMS Journal on Computing*. (LA-UR-22-25949)

Presentation Slides

Srinivasan, S. Why should you care about gradients of scalar functions of symmetric matrices ?. . (LA-UR-22-22077)

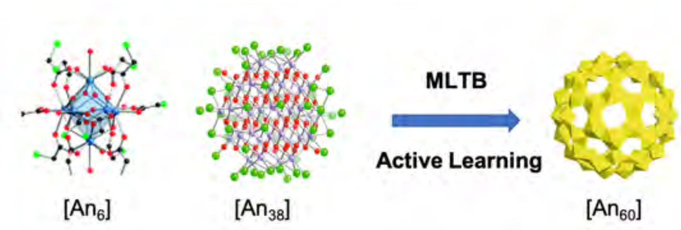
Srinivasan, S. Gas Transport Networks: Numerical Solution of Steady-State Flow Equations. . (LA-UR-22-22239)

Srinivasan, S. Gas Transport Networks: Numerical Solution of Steady-State Flow Equations. Presented at *SES 2022*, College Station, Texas, United States, 2022-10-16 - 2022-10-19. (LA-UR-22-30901)

**Peer-reviewed*

Data-driven Quantum Molecular Dynamics for Actinide Chemistry

Ping Yang
20220059ER



This project will focus on predicting nano-sized actinides clusters at the quantum-level, augmented by data-science

Project Description

This project directly addresses Department of Energy's (DOE) mission in solving the f-Element Grand Challenge and in Controlling f- Elements at the most Basic Level, that of the Electron by expanding our scientific understanding of nano-sized actinide clusters as a function of chemical matrices, pH, oxidation states of metal center, identities of anions, and organic chelates. The development of the computational methods enabling previously intractable simulations of nano-sized actinides clusters at the quantum-level will have high potential for improving predictive capability broadly for the DOE, ranging from advancing fundamental chemistry of actinides to applied areas associated with nuclear fuels, materials, and environmental remediation. Advancing our predictive capabilities in actinide structure-property relationships directly addresses the 2006 and 2017 reports on Basic Research Needs for Advanced Nuclear Energy and Future Nuclear Energy. The research described herein will enable, for the first time, capability to simulate realistic solution environments that contain actinide elements. Moreover, these results will significantly advance predictive capability relevant to technical problems associated with actinide elements, namely those associated with fuel cycles, repository science, tank waste, and plutonium processing.

Publications

Journal Articles

Taylor, M. G., D. J. Burrill, J. Janssen, E. R. Batista, D. Perez and P. Yang. Architector: high-throughput cross-periodic table 3D complex builder. Submitted to *Nature Communications*. (LA-UR-22-25834)

Presentation Slides

Taylor, M. G. Architector: towards learning across the mononuclear periodic table. Presented at *Machine Learning and Informatics for Chemistry and Materials*, Telluride, Colorado, United States, 2022-10-03 - 2022-10-07. (LA-UR-22-30196)

Taylor, M. G. Architector: high-throughput generation of f-block molecular complexes. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-03. (LA-UR-23-21730)

Taylor, M. G., D. J. Burrill, J. Janssen, E. R. Batista, D. Perez and P. Yang. Learning actinide-ligand binding motifs and structure from organometallic structural databases. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28791)

Yang, P., E. R. Batista, M. J. Cawkwell, C. Liu, R. K. Carlson, S. Wu and D. Perez. Enabling Long Time-scale Quantum Molecular Dynamics Simulations for 5f-Elements. Presented at *APATCC-10: Asian-Pacific Association of Theoretical & Computational Chemists*, Quy Nhon, Vietnam, 2023-02-19 - 2023-02-23. (LA-UR-23-21113)

**Peer-reviewed*

Quantum Computing for Flow in Complex Fracture Networks

Daniel O'Malley

20220077ER

A conceptual representation of our innovative approach to solving extremely large systems of fracture flow equations is shown. Our workflow involves three stages: (1) encoding the fracture flow equations in a way that is suitable for quantum computing (QC) at a scale that is beyond the reach of classical computing, (2) using a quantum algorithm suitable for solving extremely large systems of equations on near-term quantum computers, and (3) extracting relevant information from the flow solution, such as the pressure at well locations.

Project Description

While many challenges remain, quantum computing (QC) has shown great promise for solving problems that no classical computer can feasibly solve. However, formulating scientific problems to take advantage of QC remains elusive – details matter. Quantum speed-ups have been ruled out for many applications because large systems of equations (where QC excels) can often be replaced by small systems of equations while retaining the desired accuracy–a process called coarse-graining. Simulating fracture systems, one of the most challenging problems in geophysics, is an ideal application for quantum computers because the multiscale nature of the problem makes coarse-graining impossible. An extremely large system of equations is needed to accurately simulate a fracture system with a wide range of fracture sizes. Our goal is to exploit QC by applying it to fracture systems while simultaneously demonstrating the power of QC in the geosciences.

Publications

Journal Articles

Golden, J. K., D. O'Malley and H. S. Viswanathan. Quantum computing and preconditioners for hydrological linear systems. 2022. *Scientific Reports*. **12** (1): 22285. (LA-UR-22-24431 DOI: 10.1038/s41598-022-25727-9)

Henderson, J. M., M. Podzorova, M. V. S. Cerezo de la Roca, J. K. Golden, L. Gleyzer, H. S. Viswanathan and D. O'Malley. Quantum algorithms for geologic fracture networks. 2023. *Scientific Reports*. **13** (1): 2906. (LA-UR-22-29135 DOI: 10.1038/s41598-023-29643-4)

O'Malley, D., J. K. Golden, Y. Subasi, R. B. Lowrie and S. J. Eidenbenz. A near-term quantum algorithm for solving linear systems of equations based on the Woodbury identity. Submitted to *Quantum*. (LA-UR-22-23447)

Presentation Slides

O'Malley, D. Subsurface Flow and Transport with Differentiable Programming and Quantum Computing. Presented at *SIAM Computational Science and Engineering*, Amsterdam, Netherlands, 2023-02-27 - 2023-02-27. (LA-UR-23-22050)

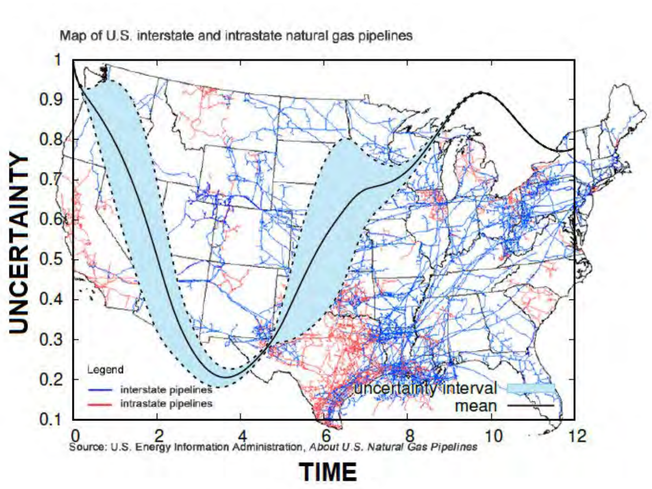
Posters

O'Malley, D. and R. Parashar. Exploring Quantum Algorithms to Determine Well Capture Zones in 2D Fractured Rock Systems. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-12. (LA-UR-22-32872)

**Peer-reviewed*

Stochastic Finite Volume Method for Robust Optimization of Nonlinear Flows

Svetlana Tokareva
20220121ER



Variation of uncertainty in energy flow as a function of time, superimposed on the complex network of pipelines in the United States. Expressing such uncertainty dynamics in optimization constraints is a grand challenge for scientific computing. The project will develop new tools for managing spatio-temporal uncertainty in complex networks. Using stochastic finite volumes to represent the evolution of uncertainty in optimization enables the precise calibration of energy flow, improving responsiveness, efficiency, and reliability of the integrated United States energy system.

Project Description

Power grids are challenged by growing use of natural gas fueled generation to balance new renewable energy sources, which are uncontrollable. This compels new methods for optimization-based pipeline operation to provide probabilistic guarantees on gas delivery. The needed robust optimization for the complex network flow physics presents mathematical and computational challenges. No robust optimization method to date can account for the space-time uncertainty that presents the major challenge for gas pipelines. We will develop the first method to manage dynamic uncertainty in constrained optimization. Conservation laws on metric graphs represent diverse phenomena such as quantum information and energy networks, and tractable uncertainty quantification in such systems remains challenging. Our method will manage uncertainty for hyperbolic balance laws that model controlled flow on networks using stochastic finite volumes (SFV). We will use the method for robust optimal control of dynamic fluid flow over energy transport networks. The project will reinforce Los Alamos National Laboratory's lead in modeling and quantifying the risks associated with complex energy systems. This capability is essential for national energy reliability and security.

Publications

Journal Articles

Tokareva, S., A. V. Zlotnik and V. Gyrya. Stochastic Finite Volume Method for Uncertainty Quantification of Transient Flow in Gas Pipeline Networks. Submitted to *Mathematical Models & Methods in Applied Sciences*. (LA-UR-22-23349)

Presentation Slides

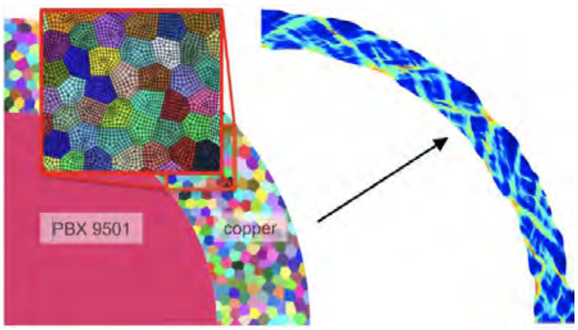
Tokareva, S., A. V. Zlotnik and V. Gyrya. Uncertainty quantification for PDEs on graphs and applications to gas networks. Presented at *SIAM Conference on Uncertainty Quantification*, Atlanta, Georgia, United States, 2022-04-12 - 2022-04-15. (LA-UR-22-23259)

Zlotnik, A. V. Stochastic Finite Volume Method for Uncertainty Quantification of Transient Flow in Gas Pipeline Networks. Presented at *SIAM Conference on Computational Science and Engineering*, Amsterdam, Netherlands, 2023-02-26 - 2023-02-26. (LA-UR-23-21491)

**Peer-reviewed*

Predictive Computational Framework for the Treatment of Dynamic Fracture Problems on Polytopal Meshes

Hashem Mourad
20220129ER



An illustrative problem of interest, involving a curved metallic shell that fragments when subjected to internal explosive loading. Correctly predicting the fragmentation pattern, fragment size distribution, etc., in a simulation of such a problem is a challenging task from both the modeling and the numerical methods perspectives. To meet this challenge, the LDRD team will develop a computational framework that represents the damage and fracture processes accurately and efficiently without introducing any artifacts that may pollute the numerical solution, taking into account relevant physical effects such as thermo-mechanical coupling in order to maximize the predictive ability of the framework.

Project Description

The failure of materials under extreme dynamic loading conditions is a central issue in many important, mission-relevant application areas. However, despite its importance, this type of material failure (dynamic fracture) is still not sufficiently well understood and cannot be reliably predicted using existing computer simulation tools. This is because experimental studies of dynamic fracture can be costly or even impossible to conduct in some cases. Moreover, analytical and computational treatments developed over the years have known shortcomings that make them difficult to implement and limit their applicability and predictive ability. To overcome these difficulties, we will develop models that represent the relevant physics in a thermodynamically consistent manner. To be able to solve the resulting equations in an accurate and efficient way, we will also develop and implement advanced numerical methods that are especially well-suited for this purpose. This treatment of fracture will be transformative given its ability to predict material damage and the subsequent initiation, propagation and branching of cracks, without any need for artificial failure criteria. This kind of predictive ability, will allow reliable high-fidelity information to be obtained from numerical simulations results, reducing reliance on expensive experimental work, in Department of Energy/ National Nuclear Security Administration mission-relevant applications.

Publications

Journal Articles

Adak, D., G. Manzini, H. M. Mourad, J. N. Plohr and L. Svolos. The C1-conforming arbitrary-order virtual element method for the two-dimensional phase-field equation. Submitted to *Journal of Scientific Computing*. (LA-UR-21-31995)

*Svolos, L., H. M. Mourad, G. Manzini and K. Garikipati. A fourth-order phase-field fracture model: Formulation and numerical solution using a continuous/discontinuous Galerkin method. 2022. *Journal of the Mechanics and Physics of Solids*. **165**: 104910. (LA-UR-21-30031 DOI: 10.1016/j.jmps.2022.104910)

Svolos, L., J. N. Plohr, G. Manzini and H. M. Mourad. On the convexity of phase-field fracture formulations: Analytical study and comparison of various degradation functions. 2023. *International Journal of Non-Linear Mechanics*. 104359. (LA-UR-22-27615 DOI: 10.1016/j.ijnonlinmec.2023.104359)

Conference Papers

Manzini, G., P. F. Antonietti, S. Scacchi and M. Verani. On arbitrarily regular conforming virtual element methods for elliptic partial differential equations. Presented at *Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2020+1: Selected Papers from the ICOSAHOM Conference*. (Vienna, Austria, 2021-08-12 - 2021-08-16). (LA-UR-21-31964)

Reports

Moutsanidis, G. and L. Svolos. Phase field modeling of dynamic brittle fracture in functionally graded materials under thermal shock. Unpublished report. (LA-UR-22-28853)

Svolos, L., G. Manzini, J. N. Plohr and H. M. Mourad. A high-regular Virtual Element Method for a fourth-order phase-field fracture model on polygonal meshes. Unpublished report. (LA-UR-21-32432)

Svolos, L., J. N. Plohr, G. Manzini and H. M. Mourad. On the stability of phase-field fracture formulations. Unpublished report. (LA-UR-22-23724)

Presentation Slides

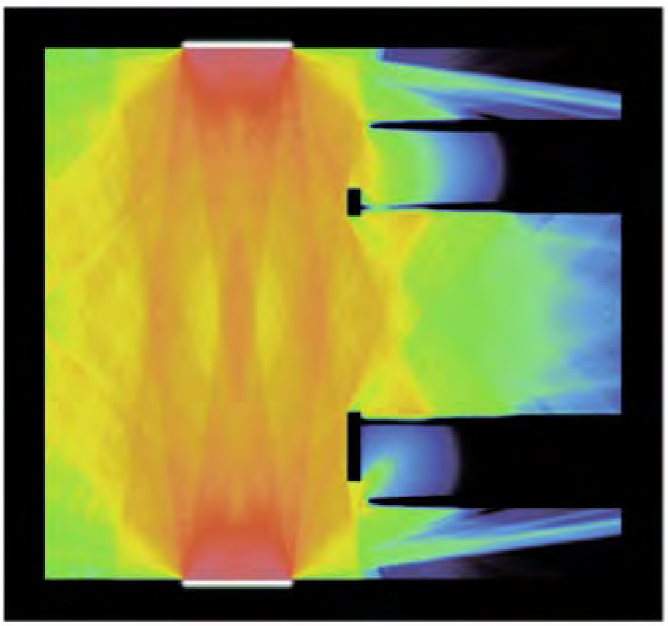
Svolos, L., H. M. Mourad, G. Manzini and K. Garikipati. A Fourth-Order Phase-Field Fracture Model: Formulation and Numerical Solution Using a Continuous/Discontinuous Galerkin Method. Presented at *Engineering Mechanics Institute Conference 2022*, Baltimore, Maryland, United States, 2022-05-31 - 2022-06-03. (LA-UR-22-24906)

Svolos, L. and H. M. Mourad. A Phase-Field Model of Ductile Fracture based on a Variational Framework for Materials with Thermo-Viscoplastic Behavior. Presented at *Society of Engineering Science Annual Technical Meeting*, College Station, Texas, United States, 2022-10-16 - 2022-10-19. (LA-UR-22-30779)

**Peer-reviewed*

High-Order Implicit-Explicit Time Integration for Radiation Transport and Coupled Multiphysics Problems

HyeongKae Park
20220174ER



This image shows a half hohlraum problem with throttled foam channels, motivated by radiation hydro- dynamics simulations for inertial confinement fusion. Problem consists of gold wall (diffusive), Tantalum wall (diffusive), and Si02 foam, and Helium fill (streaming). The figure depicts temperature profile at 1.2 ns. The algorithm to be developed in the course of this project will help address computational demanding multiphysics problems such as the half hohlraum problem above.

Project Description

This project aims to develop implicit-explicit (IMEX) time integration schemes for the numerical simulation of thermal radiative transfer (TRT) and multiphysics problems based on high-fidelity kinetic systems. The proposed IMEX approach drastically reduces the cost over implicit methods (typically used with TRT) while providing a framework for high-order accuracy and greater physics fidelity compared with traditional multiphysics operator splitting. The successful conclusion of the research proposed in this project will enable unprecedented fidelity in the modeling of the High energy density physics (HEDP) system with far fewer computational resources, thus opening a new computational frontier. The methods proposed here will also fits naturally to modern heterogeneous architectures. The algorithms stemming from this research, once successfully demonstrated, will impact a variety of mission spaces including energy security and nuclear security defense.

Publications

Journal Articles

Wimmer, G. A., B. S. Southworth, T. J. Gregory and X. Tang. A fast algebraic multigrid solver and accurate discretization for highly anisotropic heat flux I: open field lines. Submitted to *SIAM Journal on Scientific Computing*. (LA-UR-23-20885)

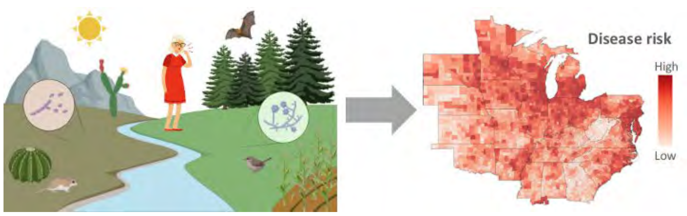
Presentation Slides

Shaw, C. A. Error study of FlecSIM using the method of manufactured solutions. . (LA-UR-22-29482)

**Peer-reviewed*

Assessing Environmental and Health Impacts of Airborne Particulates

Kimberly Kaufeld
20220209ER



Collecting disease case data is an imperfect process, especially due to limited data collection. This leads to gaps in our knowledge of disease risk. Two diseases in the United States with imperfect detection problems are Valley fever, caused by the fungus Coccidioides (left side of the river), and histoplasmosis, caused by the fungus Histoplasma (right side of the river). The goal of the project is to develop a method to fill in these gaps to more accurately understand disease risk and produce risk maps.

Project Description

In the United States, disease surveillance provides multiple datasets that make it challenging to provide nationwide disease risks. The aim of this proposal is to develop a statistical approach to incorporate varying surveillance requirements and imperfect detection of health data to assess disease risk, especially in data-sparse regions. We will develop models that account for environmental changes for two significantly underreported diseases in the United States: histoplasmosis and Valley fever using data we have obtained from the Center for Disease Control and Prevention (CDC). These two diseases are found in subsections of the US, but with changes in the environment, their geographical ranges are already both shifting and expanding. Creating a mechanism to assess the current risk of contracting these diseases from the environment now is a crucial first step for predicting which communities may be at risk in the future as the disease shifts in response to climate change. This work will result in new models for health surveillance, improving our understanding of disease spread due to differences in reporting health data, that can be readily deployed for other infectious diseases, especially at the onset of new emergent diseases or future pandemics when data collection is sparse.

Publications

Journal Articles

Gorris, M. E., K. Ardin-Dryer, A. Campuzano, L. R. Castanon-Olivares, T. E. Gill, A. D. Greene, C. Hung, K. A. Kaufeld, M. Lacy and E. Sanchez-Paredes. Advocating for coccidioidomycosis as a nationally reportable disease in the United States and encouraging disease surveillance across North and South America. Submitted to *Journal of Fungi*. (LA-UR-22-30718)

*Hepler, S. A., K. A. Kaufeld, K. Benedict, M. Toda, B. R. Jackson, X. Liu and D. Kline. Integrating Public Health Surveillance and Environmental Data to Model Presence of Histoplasma in the United States. 2022. *Epidemiology*. **33** (5): 654-659. (LA-UR-21-26964 DOI: 10.1097/EDE.0000000000001499)

Hoffman-Hall, A., M. E. Gorris, S. Anenberg, A. Bredder, J. K. Dhaliwal, M. A. Diaz, S. K. Fortner, B. McAdoo, D. Reano, R. Rehr, H. Roop and B. F. Zaitchik. A GeoHealth Call to Action: Moving Beyond Identifying Environmental Injustices to Co-Creating Solutions. 2022. *GeoHealth*. **6** (11): e2022GH000706. (LA-UR-22-28540 DOI: 10.1029/2022GH000706)

*Temple, S. D., C. A. Manore and K. A. Kaufeld. Bayesian time-varying occupancy model for West Nile virus in Ontario, Canada. 2022. *Stochastic Environmental Research and Risk Assessment*. **36** (8): 2337-2352. (LA-UR-21-31764 DOI: 10.1007/s00477-022-02257-4)

Tong, D. Q., M. E. Gorris, T. E. Gill, K. Ardon-Dryer, J. Wang and L. Ren. Dust Storms, Valley Fever, and Public Awareness. 2022. *GeoHealth*. **6** (8): e2022GH000642. (LA-UR-22-22270 DOI: 10.1029/2022GH000642)

Books/Chapters

Ebi, K. L., M. H. Hayden, M. E. Gorris, C. Uejio and J. Vanos. Chapter 15: Uncertainty in determining impacts of climate change on human health. (LA-UR-22-28552)

Presentation Slides

Gorris, M. E. Life at LANL as an Earth System Scientist, and the new field of GeoHealth. . (LA-UR-22-25545)

Gorris, M. E. The projected expansion of coccidioidomycosis (Valley fever) endemic regions in response to climate change. Presented at *ZOHU Call: Zoonoses & One Health Update*, Los Alamos, New Mexico, United States, 2022-09-07 - 2022-09-07. (LA-UR-22-29039)

Gorris, M. E. Using climate and environmental data to understand Valley fever disease dynamics. Presented at *Health Officers Association of California*, Los Alamos, New Mexico, United States, 2022-10-14 - 2022-10-14. (LA-UR-22-30977)

Gorris, M. E. Potential effects of climate change on Valley fever. Presented at *NASEM Workshop on Valley fever*, Irvine, California, United States, 2022-11-17 - 2022-11-18. (LA-UR-22-32007)

Gorris, M. E. Understanding the current and future risk of coccidioidomycosis (Valley fever). Presented at *BRaVE fungal meeting*, Los Alamos, New Mexico, United States, 2023-03-30 - 2023-03-31. (LA-UR-23-23133)

Gorris, M. E., K. A. Kaufeld, S. Hepler and D. Kline. Exploring if wildland fire activity can be a driver of Valley fever cases. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32830)

Kaufeld, K. A. Integrating public health surveillance and environmental data to model presence of Histoplasma in the United States. Presented at *BYU Seminar*, Provo, Utah, United States, 2021-11-18 - 2021-11-18. (LA-UR-21-31384)

Kaufeld, K. A. Integrating public health surveillance and environmental data to model airborne diseases\xc2\xa0in the United States. . (LA-UR-22-20612)

Kaufeld, K. A. Being a Statistician at Los Alamos National Laboratory. Presented at *SRC virtual meeting*, Virtual, New Mexico, United States, 2022-05-19 - 2022-05-19. (LA-UR-22-24669)

Kaufeld, K. A. Integrating public health surveillance and environmental data to model the presence of Histoplasma. . (LA-UR-22-29045)

Kaufeld, K. A. Integrating public health surveillance and environmental data to model fungal diseases in the United States. . (LA-UR-23-20711)

Kaufeld, K. A. A Spatio-temporal Model to Assess Environmental Impacts on Coccidioidomycosis in the Southwestern United States. Presented at *Cocci Study Group*, Tucson, Arizona, United States, 2023-03-30 - 2023-03-30. (LA-UR-23-23149)

Kaufeld, K. A. Where is the pathogenic fungus Histoplasma? An occupancy model approach for assessing the risk of histoplasmosis.. Presented at *BRaVE Planning Workshop on Aerial Dispersal*, Online, New Mexico, United States, 2023-03-30 - 2023-03-30. (LA-UR-23-23129)

Kaufeld, K. A., J. Kwon, S. Hepler, D. Kline and M. E. Gorris. A time varying occupancy model for Histoplasma in the United States. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32833)

Kaufeld, K. A., M. E. Gorris, A. D. Greene, D. Kline and S. Hepler. Integrating public health surveillance and environmental data to model the presence of Coccidioidomycosis. Presented at *66th Annual Coccidioidomycosis Study Group Meeting*, Bakersfield, California, United States, 2022-04-08 - 2022-04-09. (LA-UR-22-23216)

Kaufeld, K. A. and M. F. Dorn. Power outage forecasting for tropical cyclones. . (LA-UR-22-24037)

Kwon, J., K. A. Kaufeld and M. E. Gorris. A time-varying occupancy model for Histoplasma in the U.S. using eBird

data. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Virtual, New Mexico, United States, 2022-08-01 - 2022-08-01. (LA-UR-22-27749)

Posters

Gorris, M. E., K. A. Kaufeld, A. D. Greene, S. Hepler and D. Kline. Continued exploration of the statistical links between coccidioidomycosis cases and wildland fires. Presented at *Coccidioidomycosis Study Group 2023*, Tucson, Arizona, United States, 2023-03-31 - 2023-04-01. (LA-UR-23-23134)

Gorris, M. E., K. A. Kaufeld, S. A. Hepler and D. M. Kline. Exploring the statistical links between coccidioidomycosis cases and wildland fires. Presented at *66th Coccidioidomycosis Study Group*, Bakersfield, California, United States, 2022-04-07 - 2022-04-10. (LA-UR-22-23200)

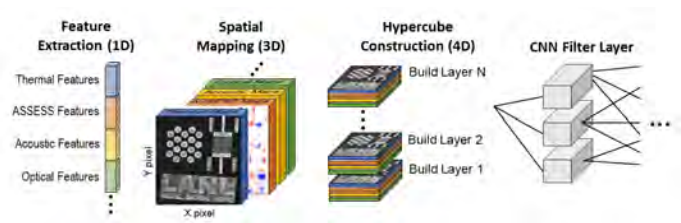
Greene, A. D., M. E. Gorris, S. A. Hepler and K. A. Kaufeld. Exploring the relationships between environmental conditions and the fungal disease blastomycosis in the midwestern United States. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-07. (LA-UR-23-22118)

Kaufeld, K. A., S. A. Hepler, M. E. Gorris, D. Kline and A. D. Greene. Integrating public health surveillance and environmental data to model the presence of Coccidioidomycosis. Presented at *Cocci Study Group*, Tucson, Arizona, United States, 2023-03-31 - 2023-04-01. (LA-UR-23-23098)

**Peer-reviewed*

Multi-Sensor Online Quality Control for Additive Manufacturing

Adam Wachtor
20220368ER



In-situ, spatially registered, multi-modal measurements made during additive manufacturing processes produce very large datasets. Associated with each pixel on each build layer is a high-dimensional stack of informational features derived from the various sensing modalities. These feature stacks for each layer will be combined over the entire build to create a 4D hypercube that will be analyzed using deep learning techniques to detect defects in additively manufactured parts.

Project Description

This work supports the qualification efforts in advanced manufacturing processes, namely additive manufacturing. Additive manufacturing is increasingly being explored as a manufacturing option for several programs within weapons and global security, because it allows the production of components with unique material properties and complex geometries without the need for significant preparation and tooling costs seen in traditional manufacturing processes. The advances of this work to predict defect populations of additively manufactured parts by combining process monitoring data streams with Los Alamos National Laboratory-developed direct part measurements made during the build process will enable the construction of a digital twin that can inform part performance modeling and acceptance.

Publications

Journal Articles

Cummings, I. T., E. M. Jacobson, E. B. Flynn, B. M. Patterson, B. K. Hunter and A. J. Wachtor. Detection of Lattice Defects in Additively Manufactured Metal Parts Using In-Situ Ultrasonic Inspection. Submitted to *Additive Manufacturing*. (LA-UR-22-22169)

Reports

Hunter, B. K. Surface Roughness Calculations of Additively Manufactured Cylinders via X-Ray Computed Tomography. Unpublished report. (LA-UR-22-22586)

Hunter, B. K. X-ray Computed Tomography as a Metrology Technique for the Analysis of Additively Manufactured Material. Unpublished report. (LA-UR-22-29166)

Shah, N. Towards Automating Registration of Laser Powder Bed Fusion Manufacturing In-situ Sensor Data and Ex-situ Identified Multiscale Defects. Unpublished report. (LA-UR-22-30294)

Presentation Slides

Patterson, B. M., B. K. Hunter, S. G. Young, T. H. Day, D. W. Schmidt and A. J. Wachtor. X-ray Tomography as a Metrology Technique. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-19. (LA-UR-23-22374)

Shah, N. Dr. Stebner Update. . (LA-UR-22-30273)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, P. J. Depond, J. Forien, G. M. Guss, N. P. Calta and M. J. Matthews. Sensor Fusion of Pyrometry and Acoustic Measurements for Localized Keyhole Pore Identification in Laser Powder Bed Fusion. . (LA-UR-22-30173)

Wachtor, A. J., J. R. Tempelman, E. B. Flynn, I. T. Cummings, E. M. Jacobson and B. M. Patterson. Defect Detection in Additively Manufactured Parts through In-Situ Monitoring and Direct-Part Inspection. Presented at *6th Cross-JOWOG Working Group Meeting on Applications, Design, and Certification of Additive Manufacturing*, Kansas City, Missouri, United States, 2022-02-28 - 2022-03-04. (LA-CP-22-20143)

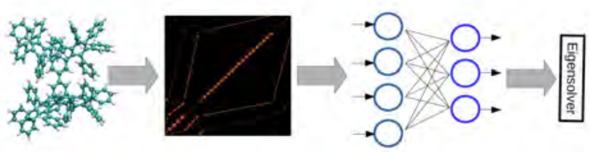
Posters

Hunter, B. K., E. M. Jacobson, I. T. Cummings, A. J. Wachtor and B. M. Patterson. X-ray Tomography as a 3D Metrology Technique for AM Materials. Presented at *Solid Freeform Fabrication Symposium*, Austin, Texas, United States, 2022-07-25 - 2022-07-27. (LA-UR-22-26980)

**Peer-reviewed*

Teaching Eigensolvers the Path to the Fastest Solution

Phillip Romero
20220428ER



The figure steps through an example problem; a sample chemical composition and its representative system matrix, and how the proposed Reinforcement Learning framework will augment a traditional Eigensolver. The goal is overall performance improvement and Floating-Point Operation (FLOP) reduction.

Project Description

Apparent in the procurement of several Exascale capable clusters e.g., El Capitan, Aurora, Frontier etc., the Department of Energy (DOE) complex is invested in the near future of classical computers. Therefore developing a faster Eigen-System solver for use in Quantum Molecular Dynamics calculations ensures that Los Alamos National Laboratory and henceforth the DOE complex satisfy the scientific readiness goals. Since a key aspect of solver design for shock physics, metal plasticity, aerodynamics etc., rely on diagonalization, the aforementioned capability will guarantee Los Alamos' competitive edge in the scientific community. An achievement of this magnitude will have massive impact in areas not limited to solver design for shock physics, metal plasticity, aerodynamics etc. as they all rely on diagonalization. Improving the efficiency of diagonalization via Machine Learning will place Los Alamos at the forefront of solver investigation as we are attempting to develop a general framework to tailor solvers to specific application.

Publications

Journal Articles

Romero, P. R., M. Bhattarai, C. F. A. Negre, A. M. Niklasson and A. A. (. Adedoyin. Teaching eigensolvers the fastest path to solution. Submitted to *IML conference journal*. (LA-UR-23-21573)

Presentation Slides

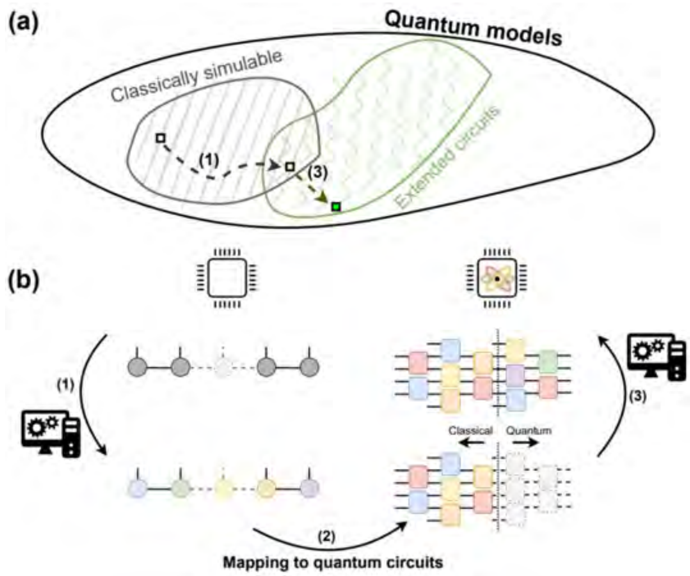
Romero, P. R., C. F. A. Negre, M. Bhattarai and A. M. Niklasson. Teaching Eigensolvers the Path to the Fastest Solution Utilizing Deep Reinforcement Learning. . (LA-UR-23-23310)

**Peer-reviewed*

Warm-Starting Quantum Machine Learning

Lukasz Cincio

20220745ER



(a) Quantum models are, in general, prohibitively hard to simulate classically. Still, for certain families of quantum states this can be achieved classically efficiently. (b) Warm-start methodology. First, a QML model is constructed based on MPS. Starting from a randomly initialized MPS an optimization involving only classical computation is performed and the best model among this restricted class, is discovered. This model is mapped to a quantum circuit which can be executed on a quantum device. Crucially, this circuit is extended such as to span a variety of models now exceeding the realm of classical simulations.

Project Description

Quantum machine learning is widely recognized as one of the best paths to achieve early quantum advantage. That is, the computational setup in which quantum computer performs a given task faster then classical computer. Success of the project's proposed work will mark one of the important milestones along the path of achieving this quantum advantage. The project team will demonstrate practical usefulness of current noisy quantum computers in mission related applications.

Publications

Journal Articles

Cincio, L., J. Cote, F. A. Sauvage, M. Larocca, M. Jonsson and T. Albash. Diabatic Quantum Annealing for the Frustrated Ring Model. Submitted to *Quantum Science & Technology*. (LA-UR-22-32570)

*Larocca, M., F. Sauvage, F. M. Sbahi, G. Verdon, P. J. Coles and M. Cerezo. Group-Invariant Quantum Machine Learning. 2022. *PRX Quantum*. **3** (3): 030341. (LA-UR-22-23371 DOI: 10.1103/PRXQuantum.3.030341)

S. Cerezo de la Roca, M. V., L. Schatzki, M. Larocca and F. A. Sauvage. Theoretical Guarantees for Sn-Equivariant Quantum Neural Networks. Submitted to *Nature Communications*. (LA-UR-22-29899)

S. Cerezo de la Roca, M. V., M. Ragone, P. Braccia, Q. T. Nguyen, L. Schatzki, P. J. Coles, F. A. Sauvage and M. Larocca. Representation Theory for Geometric Quantum Machine Learning. Submitted to *Quantum*. (LA-UR-22-30670)

S. Cerezo de la Roca, M. V., Q. T. Nguyen, L. Schatzki, P. Braccia, M. Ragone, P. J. Coles, F. A. Sauvage and M. Larocca. Theory for Equivariant Quantum Neural Networks. Submitted to *Physical Review X*. (LA-UR-22-30859)

Sauvage, F. A., M. Larocca, P. J. Coles and M. V. S. Cerezo de la Roca. Building spatial symmetries into parameterized quantum circuits for faster training. Submitted to *Quantum*. (LA-UR-22-27391)

Conference Papers

Sauvage, F. A., Q. Nguyen, L. M. Schatzki, P. Braccia, M. J. Ragone, P. J. Coles, M. Larocca and M. V. S. Cerezo de la Roca. A Theory for Equivariant Quantum Neural Networks. Presented at *Quantum information Processing*. (Ghent, Belgium, 2023-02-04 - 2023-02-10). (LA-UR-22-29896)

Presentation Slides

Sauvage, F. A., M. Larocca, P. J. Coles and M. V. S. Cerezo de la Roca. Building spatial symmetries into parameterized quantum circuits for faster training. Presented at *SQUINT 24th edition*, Berkeley, California, United States, 2022-10-20 - 2022-10-22. (LA-UR-22-30936)

Sauvage, F. A., M. Larocca, P. J. Coles and M. V. S. Cerezo de la Roca. Building spatial symmetries into parameterized quantum circuits for faster training. Presented at *Quantum Techniques in Machine Learning (QTML)*, Naples, Italy, 2022-11-07 - 2022-11-12. (LA-UR-22-31694)

Sauvage, F. A., M. Larocca, Q. Nguyen, L. M. Schatzki, M. J. Ragone, F. M. Sbahi, G. Verdon, P. J. Coles and M. V. S. Cerezo de la Roca. Towards Geometric Quantum Machine Learning. . (LA-UR-22-32571)

**Peer-reviewed*

Quantification of T-Cell Receptor Cross-Reactivity: Immunology Meets Network Theory

Sidhant Misra
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Figure is of a bipartite network representing T cell receptor cross-reactivity. An edge in the network indicates whether a given TCR (with alpha and beta chains) recognizes an epitope. The network provides a mathematical means to analyze the behavior of T cell immunity. Due to scarcity of experimental data, many edges in the network are unknown. Machine learning techniques will be able to predict missing edges, assess the confidence of predicted edges and inform future experiment design for maximizing information. Figure reproduced from Bentzen and Hadrup (2019), Immuno-Oncology Technology, T cell receptor cross-recognition and strategies to select safe T cell receptors for clinical translation.

Project Description

The project addresses challenges in bio-security and health by development of mathematical models and methods to understand the behavior of T lymphocyte (T cells) and cross-reactivity. By using machine learning techniques, the project aims to develop novel tools and metrics that can be used to better understand properties of T cell immunity such as cross-reactivity. These tools will be provide a means to analyze available immunological data sets and inform future immunological experiment design. Ultimately, these methods can help enhance our understanding of T cell immune responses to viral infections and cancers, and the design of a future universal influenza vaccine.

Publications

Presentation Slides

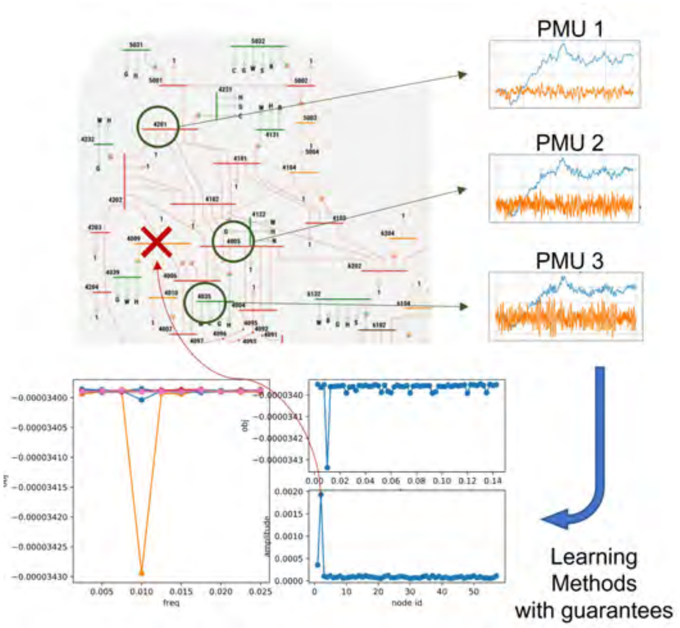
Molina-Paris, C. Modelling within-host and population level infection dynamics: Multi-scale within-host immuno-epi. . (LA-UR-22-30416)

Molina-Paris, C. and G. Lythe. Stochastic and deterministic models in immunology Thymic selection, homeostasis of naive T cells and compartments. Presented at *Summer School in Sao Paulo*, Sao Paulo, Brazil, 2022-11-07 - 2022-11-11. (LA-UR-22-31733)

**Peer-reviewed*

Locating Forced Oscillations in Power Networks

Marc Vuffray
20220774ER



By observing at various locations the dynamic of complex networks (here a power grid), a perturbation (shown in red) caused by a malfunctioning component is detected and localized before it can damage the integrity of the network thanks to our newly developed algorithm.

Project Description

One of the core missions of the Department of Energy is to ensure safe and reliable energy delivery across the United States. The outcomes of this project will lead to new ways to find undesirable sources of perturbations that are detrimental to the lifespan of vital assets in critical infrastructure networks such as power transmission and distribution grids and natural gas networks. This challenge is especially important to tackle today for the increasing penetration of renewable energy in our energy delivery networks introduces more source of uncertainty and perturbations.

Publications

Journal Articles

Delabays, R., A. Lokhov, M. S. Tyloo and M. D. Vuffray. Locating the source of forced oscillations in transmission power grids. Submitted to *Nature Energy*. (LA-UR-22-32412)

Tyloo, M. S. Faster network disruption from layered oscillatory dynamics. 2022. *Chaos: An Interdisciplinary Journal of Nonlinear Science*. **32** (12): 121102. (LA-UR-22-30194 DOI: 10.1063/5.0129123)

Conference Papers

Tyloo, M. S. Assessing the impact of Byzantine attacks on coupled phase oscillators. Presented at *IEEE Conference on Decision and Control*. (Singapore, Singapore, 2023-12-13 - 2023-12-15). (LA-UR-23-23095)

Presentation Slides

Lokhov, A. Locating the source of forced oscillations in transmission power grids. Presented at *Grid Science Winter School and Conference*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-09. (LA-UR-23-20309)

Tyloo, M. S. Noise Transmission in Layered Complex Networks. Presented at *COMPLEX NETWORKS 2022 The 11th International Conference on Complex Networks and their Applications*, Palermo, Italy, 2022-11-08 - 2022-11-10. (LA-UR-22-30069)

Tyloo, M. S. Noise Transmission and Disruption in Layered Complex Networks. Presented at *Visit University of Naples Federico II, Italy*, Naples, Italy, 2022-11-11 - 2022-11-16. (LA-UR-22-31747)

Tyloo, M. S. Locating the source of forced oscillations in complex oscillator networks and power grids. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-21609)

Posters

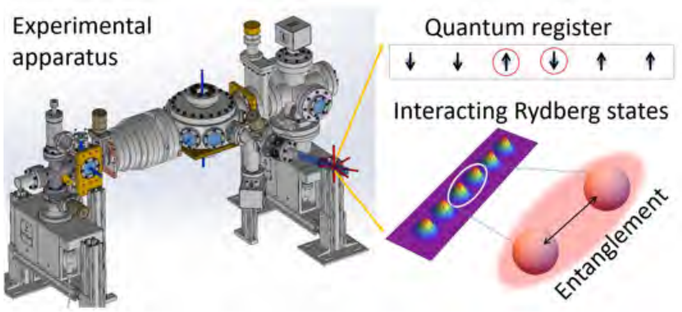
Delabays, R., A. Lokhov, M. S. Tyloo and M. D. Vuffray. Locating the source of forced oscillations in transmission grids. Presented at *gridscience*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-13. (LA-UR-22-32849)

Tyloo, M. S. Fluctuations in Layered Complex Networks. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-02-10. (LA-UR-23-21608)

**Peer-reviewed*

Quantum Computing with Strontium Nuclear Qubits

Michael Martin
20200015ER



The goal of the experimental apparatus (left panel) is to cool strontium-87 atoms to a millionth of a degree above absolute zero. This project explores the capability of using such tweezer-trapped strontium-87 to demonstrate a high-quality qubit, with quantum information stored in the nuclear spin degrees of freedom. Optical tweezers trap individual atoms and move them into laser interaction regions where internal degrees of freedom are manipulated and entangled via exciting to Rydberg states (states where an electron occupies a high-lying orbital, bottom right). The project team will further explore the unique capabilities enabled by utilizing all 10 nuclear spin degrees of freedom.

Project Description

The subcommittee on Quantum Information Science under the Committee on Science of the National Science and Technology Council published a report in September 2018 entitled "National Strategic Overview for Quantum Information Science." Here, the economic and defense implications of developing a quantum computer are discussed. Cited applications included optimization problems, chemistry, and machine learning. Meanwhile, there is a vast gap between the capabilities of current quantum hardware and the hardware requirements of useful quantum algorithms. For example, chemistry calculations can require qubit numbers of 10,000 to 1,000,000, corresponding to error rates at the part-per-billion to part-per-thousand level, respectively (smaller error rates require fewer qubits). Therefore, an outstanding challenge is to chart a path towards these kinds of performance specifications, the realization of which may be decades in the making. Neutral atom systems, as developed here, are one promising approach. This work will explore a system comprising interacting qubits encoded in the nucleus of the alkaline earth atom strontium, which has already been extensively studied in the field of atomic clocks. The same properties that makes strontium a good atomic clock can also yield good qubits, and we will explore the fundamental interactions and limitations in a few-qubit system.

Technical Outcomes

This project established experimental capabilities for using strontium-based qubits, including an ultra-high vacuum system. The team did not demonstrate qubits by the conclusion of the project, but the required hardware. The team demonstrated numerically that all 10 spin states in strontium-87 are useful for storing quantum information, going beyond the initial goal of qubits. The team also showed entangling operations between different atoms with d-dimensional nuclear-spin registers ("qudits") are possible by exciting to Rydberg levels.

Publications

Journal Articles

*Mitra, A., M. J. Martin, G. W. Biedermann, A. M. Marino, P. M. Poggi and I. H. Deutsch. Robust M\xc3\xb8lmer-S \xc3\xb8rensen gate for neutral atoms using rapid adiabatic Rydberg dressing. 2020. *Physical Review A*. **101** (3): 030301. (LA-UR-19-31221 DOI: 10.1103/PhysRevA.101.030301)

Mitra, A., S. Omanakuttan, M. J. Martin, G. Biedermann and I. Deutsch. Practical and fundamental limits of neutral atom entanglement using Rydberg dressing. Submitted to *Physical Review A*. (LA-UR-22-24775)

Omanakuttan, S., A. Mitra, M. J. Martin and I. Deutsch. Qudit entanglers using quantum optimal control. Submitted to *PRX Quantum*. (LA-UR-22-33002)

*Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum optimal control of ten-level nuclear spin qudits in 87Sr. 2021. *Physical Review A*. **104** (6): L060401. (LA-UR-21-25988 DOI: 10.1103/PhysRevA.104.L060401)

Schine, N., A. Young, W. Eckner, M. J. Martin and A. Kaufman. Long-lived Bell states in an array of optical clock qubits. Submitted to *Nature Physics*. (LA-UR-21-29502)

Presentation Slides

Martin, M. J. Quantum information science with Rydberg atoms. . (LA-UR-20-29116)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *UNM CQuIC seminar*, Albuquerque, New Mexico, United States, 2021-02-04 - 2021-02-04. (LA-UR-21-20920)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *LANL/TAMU Quantum Seminar Series*, College Station, Texas, United States, 2021-04-27 - 2021-04-27. (LA-UR-21-23972)

Martin, M. J. Quantum information science and sensing with ultracold neutral atoms. . (LA-UR-21-25997)

Martin, M. J. Quantum information science with laser-dressed atoms Q-SEnSE Convergence Seminar. Presented at *Q-SEnSE Convergence Seminar*, Boulder, Colorado, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32107)

Martin, M. J. Ultracold atom-based quantum technologies at LANL. Presented at *RPI/LANL Nucleation Workshop on Quantum Materials and Devices*, Los Alamos, New Mexico, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-23851)

Martin, M. J. Microscopic control of entanglement. Presented at *Q-SEnSE Annual Meeting*, Boulder, Colorado, United States, 2022-06-30 - 2022-07-01. (LA-UR-22-26122)

Martin, M. J. Microscopic control of entanglement. Presented at *Q-SEnSE NSF Site visit*, Boulder, Colorado, United States, 2022-08-16 - 2022-08-17. (LA-UR-22-28659)

Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

de Melo, L. F., E. J. Meier and M. J. Martin. Neutral Atom Quantum Information Science. Presented at *EMC3 Workshop*, Spring, Texas, United States, 2022-12-06 - 2022-12-07. (LA-UR-22-32645)

de Melo, L. F., T. M. Bersano, E. J. Meier, H. P. Lamsal, A. K. Harter, A. Mitra, S. Omanakuttan, I. Deutsch and M. J. Martin. Optical tweezer experiments at Los Alamos National Laboratory. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-30 - 2022-06-03. (LA-UR-22-24820)

Mitra, A., S. Omanakuttan, M. J. Martin, G. Biedermann and I. Deutsch. Fundamental and technical aspects of neutral atom entanglement via adiabatic Rydberg dressing. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-30 - 2022-06-03. (LA-UR-22-24807)

Mitra, A., S. T. Omanakuttan, M. J. Martin, G. W. Biedermann and I. H. Deutsch. Fundamental limits of neutral atom entanglement using Rydberg dressing. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, College Park, Maryland, United States, 2021-05-31 - 2021-06-04. (LA-UR-21-25172)

Omanakuttan, S., A. Mitra, I. H. Deutsch and M. J. Martin. Quantum control of nuclear spins. Presented at *APS Four Corners Meeting*, Albuquerque, New Mexico, United States, 2020-10-23 - 2020-10-24. (LA-UR-20-28577)

Omanakuttan, S., A. Mitra, M. J. Martin and I. Deutsch. Qudit entanglers using quantum control on nuclear-spin qudits. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22133)

Omanakuttan, S., A. Mitra, M. J. Martin and I. Deutsch. Qudit entanglers using quantum optimal control and Rydberg interaction on nuclear-spin qudits. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-30 - 2022-06-03. (LA-UR-22-24808)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Control of Nuclear Spin for Quantum Logic with Qudits. Presented at *APS March Meeting*, College Park, Maryland, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22461)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Control of Nuclear Spin for Quantum Logic with Qudits. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, College

Park, Maryland, United States, 2021-05-31 - 2021-06-04. (LA-UR-21-25168)

Posters

Segura Carrillo, E. A. Developing Blue-Detuned Optical Bottle Beams for Cold Rydberg Atom Technologies. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-02. (LA-UR-22-27899)

Segura Carrillo, E. A. Developing Blue-Detuned Optical Bottle Beams for Cold Rydberg Atom Technologies. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-29351)

de Melo, L. F., T. M. Bersano, E. J. Meier, H. P. Lamsal, A. K. Harter, S. Omanakuttan, A. Mitra, I. Deutsch and M. J. Martin. Optical tweezer experiments at Los Alamos National Laboratory. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-30 - 2022-06-03. (LA-UR-22-24752)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Optimal Control of Nuclear Spin Qudecimals in 87Sr. Presented at *Q-SEnSE Annual Meeting*, Boulder, Colorado, United States, 2021-07-20 - 2021-07-21. (LA-UR-21-26508)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Implementing qudit quantum logic gates on nuclear spins in 87Sr. Presented at *Southwest Quantum Information and Technology Workshop*, Albuquerque, New Mexico, United States, 2021-10-14 - 2021-10-15. (LA-UR-21-30066)

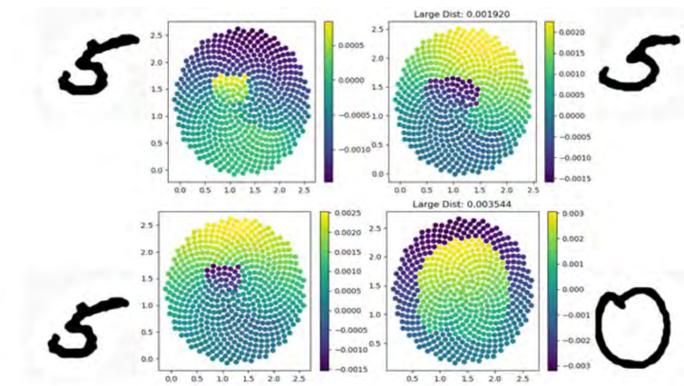
Other

Segura Carrillo, E. A. Pictures of BoB Experiment for LANL Article. Audio/Visual. (LA-UR-22-31108)

**Peer-reviewed*

Topological Relation-Based Image Analysis using Graphs

Diane Oyen
20200041ER



Graphs represent shape and spatial information in drawings and other technical images so that similar objects, like the handwritten numerals "5", have similar graphs.

Project Description

The analysis of technical imagery is critical to matters of national security, including tracking the sharing of technical diagrams for nuclear counterproliferation, quantifying the shapes of components in images of electronics for homeland security, and in quantifying shapes of particles in materials imaging for nuclear forensics. Computer vision, especially through the use of machine learning methods, has dramatically improved the ability to detect objects in images. However, these advances have not yet automated the understanding of information contained in hand-drawn figures, technical diagrams, and imagery produced for scientific inquiry. Our key innovation is the insight that these technical images carry little per pixel information compared with natural images (photographs and video), and that context, topology and shape provide information. By representing images as hierarchical graphs, with annotations on topological relationships, we will model the context and knowledge necessary to perform intelligent analysis of images. We will be able to find altered copies of technical diagrams, whether being shared online or in publications; match tomography images to databases of known commercial electronics; and identify common shapes in materials images for forensics.

Technical Outcomes

The project successfully achieved the goal of retrieving images with similar shape and finding altered copies of technical diagrams. To accomplish this, the team collected over 300,000 technical drawings from the United States patent office. An unexpected achievement is that the project team was able to train machine learning algorithms to perform better than prior methods on the computer vision tasks of retrieving images by shape.

Publications

Journal Articles

Scott, C., E. Mjolsness, D. A. Oyen, C. Kodera, M. Uyttewaal and D. Bouchez. Graph Metric Learning Quantifies Morphological Differences between Two Genotypes of Shoot Apical Meristem Cells in Arabidopsis. 2023. *in silico Plants*. (LA-UR-23-20347 DOI: 10.1093/insilicoplants/diad001)

Conference Papers

Ajayi, K., X. Wei, M. Gryder, W. Shields, J. Wu, S. M. Jones, M. Kucer and D. A. Oyen. DeepPatent2: A Large-Scale Benchmarking Corpus for Technical Drawing Understanding. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*. (New Orleans, Louisiana, United States, 2022-11-29 - 2022-11-29). (LA-UR-22-26027)

Bhattarai, M., D. A. Oyen, J. E. Castorena, L. Yang and B. E. Wohlberg. Diagram Image Retrieval using Sketch-Based Deep Learning and Transfer Learning. Presented at *CVPR DIRA Workshop*. (Seattle, Washington, United States, 2020-06-14 - 2020-06-14). (LA-UR-20-22562)

Castorena, J. E., D. A. Oyen and M. Bhattarai. Learning Spatial Relationships between Samples of Image Shapes. Presented at *Conference on Computer Vision and Pattern Recognition*. (Seattle, Washington, United States, 2020-06-14 - 2020-06-19). (LA-UR-20-22517)

Castorena, J. E. and D. A. Oyen. Learning Shapes on Image Sampled Points with Dynamic Graph CNNs. Presented at *IEEE SSIAI 2020*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29). (LA-UR-20-24122)

Gong, M., L. Yang, C. G. Potts, D. A. Oyen, B. E. Wohlberg and V. K. Asari. TGGLines: A Robust Topological Graph Guided Line Segment Detector for Low Quality Binary Images. Presented at *CVPR 2020*. (Seattle, Washington, United States, 2020-06-13 - 2020-06-20). (LA-UR-19-31578)

Gong, M., X. Wei, D. A. Oyen, J. Wu, M. Gryder and L. Yang. Recognizing Figure Labels in Patents. Presented at *AAAI Workshop on Scientific Document Understanding*. (Online, New Mexico, United States, 2021-02-02 - 2021-02-02). (LA-UR-20-29690)

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval. Presented at *Winter Application on Computer Vision*. (Waikoloa, Hawaii, United States, 2022-01-04 - 2022-01-08). (LA-UR-21-28183)

Kucer, M. and D. A. Oyen. DeepPatent: large scale patent image recognition and retrieval. Presented at *Computer Vision and Pattern Recognition (CVPR) 2021*. (Virtual, New Mexico, United States, 2021-06-19 - 2021-06-19). (LA-UR-20-29372)

Kucer, M. and D. A. Oyen. DeepPatent: Large scale patent image recognition and retrieval. Presented at *International Conference on Computer Vision 2021*. (Montreal, Canada, 2021-10-10 - 2021-10-17). (LA-UR-21-22455)

Kucer, M. and D. A. Oyen. Transfer Learning with fewer ImageNet classes. Presented at *021 Conference on Neural Information Processing Systems*. (Sydney, Australia, 2021-12-06 - 2021-12-14). (LA-UR-21-29446)

Oyen, D. A., M. Kucer and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *SPIE Conference on Machine Learning*. (San Diego, California, United States, 2021-08-03 - 2021-08-03). (LA-UR-21-27432)

Oyen, D. A., M. L. Dubey and M. Kucer. Duplicate Image Detection for Fast Identification of Easily-Confused Classes in ImageNet. Presented at *NeurIPS Workshop on ImageNet*. (Virtual, New Mexico, United States, 2021-12-13 - 2021-12-13). (LA-UR-21-29269)

Oyen, D. A. and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *Workshop on Applications of Computer Vision*. (Virtual, New Mexico, United States, 2021-01-05 - 2021-01-05). (LA-UR-20-27837)

Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodama, D. Bouchez and M. Uyttewaal. Diff2Dist: Differentiable Graph Diffusion Distance. Presented at *The Sixth International Workshop on Deep Learning on Graphs: Methods and Applications*. (Singapore, Singapore, 2021-08-14 - 2021-08-14). (LA-UR-21-24905)

Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodera, M. Uyttewaal and D. Boucher. Diff2Dist: Learning Spectrally Distinct Edge Functions, with Applications to Cell Morphology Analysis. Presented at *German Conference on Pattern Recognition*. (Online, Germany, 2021-09-28 - 2021-09-28). (LA-UR-21-25927)

Wei, X., J. Wu, K. Ajayi and D. A. Oyen. Visual Descriptor Extraction from Patent Figure Captions: A Case Study of Data Efficiency Between BiLSTM and Transformer. Presented at *JCDL*. (Cologne, Germany, 2022-06-20 - 2022-06-20). (LA-UR-22-23565)

Presentation Slides

Bhattarai, M., D. A. Oyen, J. E. Castorena, L. Yang and B. E. Wohlberg. Diagram Image Retrieval using Sketch-Based Deep Learning and Transfer Learning. Presented at *Diagram Image Retrieval and Analysis (DIRA): Representation, Learning, and Similarity Metrics*, Seattle, Washington, United States, 2020-06-14 - 2020-06-16. (LA-UR-20-23817)

Castorena, J. E., D. A. Oyen and M. Bhattarai. Learning Spatial Relationships between Samples of Patent Image Shapes. Presented at *IEEE Computer Vision and Pattern Recognition*, Seattle, Washington, United States, 2020-06-14 - 2020-06-14. (LA-UR-20-24123)

Castorena, J. E. and D. A. Oyen. Learning Shapes on Image Sampled Points with Dynamic Graph CNNs. Presented

at *2020 IEEE Southwest Symposium on Image Analysis and Interpretation*, Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29. (LA-UR-20-24124)

Gong, M., X. Wei, D. A. Oyen, J. Wu, M. Gryder and L. Yang. Recognizing Figure Labels in Patents. Presented at *AAAI Workshop on Scientific Document Understanding*, Online, New Mexico, United States, 2021-02-09 - 2021-02-09. (LA-UR-21-21174)

U. Hoque, M. R., D. A. Oyen and J. Wu. Segmenting Technical Drawing Figures in US Patents. Presented at *LANL Student Symposium*, Virtual, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27599)

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval. Presented at *Winter Application on Computer Vision 2022*, Waikoloa, Hawaii, United States, 2022-01-04 - 2022-01-08. (LA-UR-21-32274)

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval - dataset and a trained model. Presented at *WACV*, Waikoloa, Hawaii, United States, 2022-01-03 - 2021-12-08. (LA-UR-21-32339)

Oyen, D. A. Image Signatures for Diagram Image Retrieval. Presented at *Southwest Symposium on Image Analysis and Interpretation*, Santa Fe, New Mexico, United States, 2020-03-30 - 2020-03-30. (LA-UR-20-22595)

Oyen, D. A., J. E. Castorena, B. E. Wohlberg, L. Yang, M. Gong, C. Potts and M. Bhattarai. GoFigure: Tracking the Dissemination of Technical Information in Images. Presented at *DHS Science and Technology Symposium*, Washington, District Of Columbia, United States, 2020-07-13 - 2020-07-13. (LA-UR-20-25121)

Oyen, D. A., M. Kucer and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *SPIE Machine Learning*, San Diego, California, United States, 2021-08-01 - 2021-08-01. (LA-UR-21-26622)

Oyen, D. A., M. Kucer and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *SPIE Machine Learning*, San Diego, California, United States, 2021-08-01 - 2021-08-01. (LA-UR-21-26662)

Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodera, D. Bouchez and M. Uttyewaal. Diff2Dist: Differentiable Graph Diffusion Distance. Presented at *Knowledge Discovery and Data Mining*, Virtual, New Mexico, United States, 2021-08-14 - 2021-08-14. (LA-UR-21-27979)

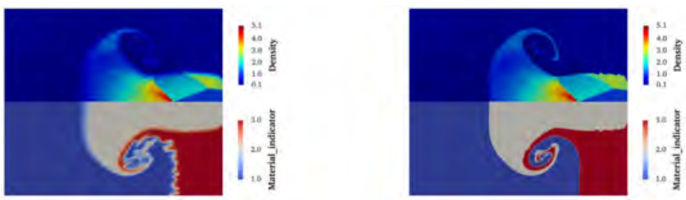
Posters

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval. Presented at *Winter Application on Computer Vision 2022*, Waikoloa, Hawaii, United States, 2022-01-04 - 2022-01-08. (LA-UR-21-31913)

**Peer-reviewed*

Adaptive High-Order Finite Element Arbitrary Lagrangian-Eulerian (ALE) Methods for Multi-Material Hydrodynamics

Aditya Kiran Pandare
20200201ER



Sharp numerical interface capturing is a key ingredient of any numerical method for multi-material hydrodynamics and multiple LANL mission areas. Pictured is an example improvement (from left to right) in bulk density and material indicator for the triple-point problem, a well-known test case for multi-material hydrodynamics schemes without (left) and with (right) our newly developed sharp-interface treatment. The figure on the right represents non-diffusive interfaces more accurately because the material interfaces are sharper. The simulation was performed in 3D and in parallel and thus its implementation is immediately useful in production, computing engineering problems.

Project Description

This research improves the accuracy, fidelity, and efficiency of, and therefore increases our trust in, the numerical simulation of multi-material hydrodynamics, which is a critical ingredient of multiple Laboratory/Department of Energy (DOE) and National Nuclear Security Administration (NNSA) programs. This work will establish the applicability of a heretofore unexplored combination of modern and adaptive numerical methods for multi-material problems combined with automatic load balancing that also enables efficient use of supercomputing hardware. This project also addresses multiple shortcomings in the current state of-practice by using modern numerical methods, previously unexplored in the context of multi-material flows at Los Alamos National Laboratory, in academia, or industry.

Technical Outcomes

The team developed a new accurate and efficient numerical method for multi-material hydrodynamics. They utilized, and thus established the applicability of, p-adaptive high-order methods for multi-material problems in an unsplit formulation, to address several shortcomings in the state-of-practice. Combining adaptation and automatic load balancing yielded up to 5X savings in costs. Furthermore, exact solutions for these equations were derived, which did not exist in literature, enabling thorough verification of multi-material numerical methods.

Publications

Journal Articles

Li, W., A. K. Pandare, H. Luo, J. Bakosi and J. I. Waltz. A Parallel p-adaptive Discontinuous Galerkin Method for the Euler Equations with Dynamic Load-Balancing on Tetrahedral Grids. Submitted to *Computers & Fluids*. (LA-UR-21-24430)

Pandare, A. K., J. I. Waltz, W. Li, H. Luo and J. Bakosi. On the Design of Stable, Consistent, and Conservative High-Order Methods for Multi-Material Hydrodynamics. Submitted to *Journal of Computational Physics*. (LA-UR-22-31308)

*Pandare, A. K., J. Waltz and J. Bakosi. Multi-material hydrodynamics with algebraic sharp interface capturing. 2021. *Computers & Fluids*. **215**: 104804. (LA-UR-20-25462 DOI: 10.1016/j.compfluid.2020.104804)

Conference Papers

Li, W., H. Luo, A. K. Pandare and J. Bakosi. A p-adaptive Discontinuous Galerkin Methods for Compressible Flows Using CHARM++. Presented at *AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-20-27898)

Pandare, A. K., J. I. Waltz and J. Bakosi. A Discontinuous Galerkin method for Non-Equilibrium Multi-Material Flows on Unstructured Grids. Presented at *AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-32156)

Pandare, A. K., J. I. Waltz and J. Bakosi. Algebraic sharp interface capturing for non-equilibrium multi-material flows. Presented at *AIAA SciTech 2021 Forum*. (Nashville, Tennessee, United States, 2021-01-11 - 2021-01-21). (LA-UR-20-29614)

Pandare, A. K., W. Li, J. I. Waltz, H. Luo and J. Bakosi. Discontinuous Galerkin Methods for Multi-Material Shock Hydrodynamics. Presented at *International conference on computational fluid dynamics (ICCFD11)*. (Maui, Hawaii, United States, 2022-07-11 - 2022-07-15). (LA-UR-22-25461)

Pandare, A. K., W. Li, J. I. Waltz, J. Bakosi and H. Luo. A THINC-DG Method for Multi-Material Fluid Flow. Presented at *AIAA SciTech Forum 2022*. (San Diego, California, United States, 2022-01-03 - 2022-01-07). (LA-UR-21-31586)

Reports

Pandare, A. K. Adaptive high-order finite element ALE methods for multi-material hydrodynamics. Unpublished report. (LA-UR-22-29840)

Presentation Slides

Pandare, A. K., J. I. Waltz and J. Bakosi. A DG Method for Non-Equilibrium Multi-Material Flows on Unstructured Grids. Presented at *AIAA SciTech Forum 2020*, Orlando, Florida, United States, 2020-01-06 - 2020-01-10. (LA-UR-20-20119)

Pandare, A. K., J. I. Waltz and J. Bakosi. Algebraic sharp interface capturing for non-equilibrium multi-material flows. Presented at *AIAA SciTech 2021 Forum*, Nashville, Tennessee, United States, 2021-01-11 - 2021-01-11. (LA-UR-20-29855)

Pandare, A. K., W. Li, J. I. Waltz, H. Luo and J. Bakosi. DG Methods for Multi-Material Shock Hydrodynamics. Presented at *International Conference on Computational Fluid Dynamics*, Maui, Hawaii, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26256)

Pandare, A. K., W. Li, J. I. Waltz, J. Bakosi and H. Luo. A THINC-DG Method for Multi-Material Flow. Presented at *AIAA Scitech 2022 Forun*, san diego, California, United States, 2022-01-03 - 2022-01-03. (LA-UR-21-31796)

Waltz, J. I., A. K. Pandare, J. Bakosi, W. Li and H. Luo. Adaptive high-order finite element ALE methods for multi-material hydrodynamics. . (LA-UR-21-23483)

**Peer-reviewed*

Sampling the Unknown: Robust Modeling of Atomic Potentials

Kipton Barros
20200209ER

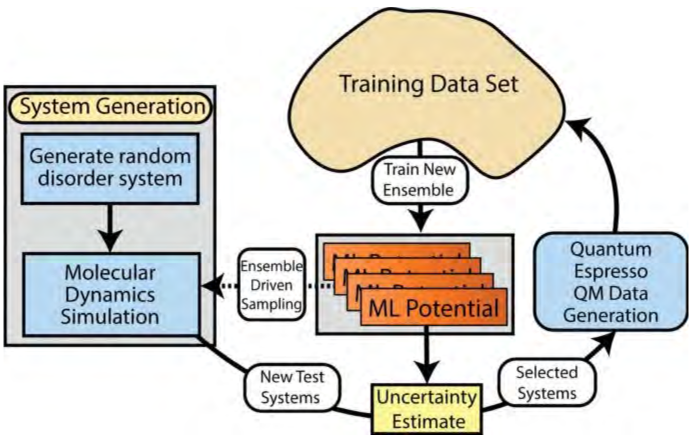


Illustration of the active learning workflow being developed in the current project. The goal is to produce machine learning (ML) potentials to predict interatomic energies and forces. The ML models are be trained from a dataset of high-quality quantum mechanical (QM) calculations. Molecular dynamics simulations are performed to generate new atomic configurations. If the ML model reports a large uncertainty on a given configuration, that configuration is selected for data generation using a new QM calculation. An innovation in the present work is to directly bias the molecular dynamics sampling towards configurations with large uncertainty.

Project Description

Machine Learning (ML) is revolutionizing the field of interatomic potential development. If successful, this project will produce a collection of methodologies for fully automated development of ML-based interatomic potentials, with robust density functional theory (DFT)-level accuracies and transferability to a broad range of physical processes. The cost of our force calculations scales linearly with system size, and the prefactor is about 100x that of classical potentials. At the end of this project, we anticipate that our distributed and graphics processing unit (GPU)-optimized ML codes will enable the simulation of millions of atoms with DFT-level accuracy.

Technical Outcomes

This project achieved significant progress in the development of methodologies for the machine learning potentials to enable atomistic simulations. The team explored the idea of "biasing towards uncertainty" to improve the effectiveness of active learning, in which the machine learning model plays a role in the collection of training data. Technical work was disseminated through authorship of 16 scientific articles, and improved machine learning architectures.

Publications

Journal Articles

Barros, K. M., M. Shahzad and S. H. Curnoe. Phase Diagram of a Spin-ice Kondo Lattice Model in the Breathing Pyrochlore Lattice. Submitted to *Physical Review B*. (LA-UR-20-25625)

*Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. 2020. *The Journal of Chemical Physics*. **153** (10): 104502. (LA-UR-19-31421 DOI: 10.1063/5.0017894)

*Craven, G. T., N. Lubbers, K. Barros and S. Tretiak. Determination of Structural Correlation Functions. 2020. *The Journal of Physical Chemistry Letters*. **11** (11): 4372-4378. (LA-UR-19-32446 DOI: 10.1021/acs.jpclett.0c00627)

Dahlbom, D., C. Miles, H. Zhang, C. D. Batista and K. M. Barros. Langevin dynamics of generalized spins as SU(N) coherent states. Submitted to *Physical Review B*. (LA-UR-22-29204)

Gao, X., F. Ramezanghorbani, J. S. Smith and A. E. Roitberg. TorchANI: A Free and Open Source PyTorch Based Deep Learning Implementation of the ANI Neural Network Potentials. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22710)

Gupta, P. L., J. S. Smith and A. E. Roitberg. Rationalizing the pH-activity response of Escherichia coli glycinamide ribonucleotide transformylase through computational methods. Submitted to *Journal of Physical Chemistry B*. (LA-UR-21-21573)

Klein, W., H. Gould and S. Matin. Cluster Scaling and Critical Points: A Cautionary Tale. Submitted to *Physical Review Letters*. (LA-UR-22-26384)

*Kulichenko, M., J. S. Smith, B. Nebgen, Y. W. Li, N. Fedik, A. I. Boldyrev, N. Lubbers, K. Barros and S. Tretiak. The Rise of Neural Networks for Materials and Chemical Dynamics. 2021. *The Journal of Physical Chemistry Letters*. **12** (26): 6227-6243. (LA-UR-21-23254 DOI: 10.1021/acs.jpclett.1c01357)

Kulichenko, M., K. M. Barros, N. E. Lubbers, Y. W. Li, R. A. Messerly, S. Tretiak, J. S. Smith and B. T. Nebgen. Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials. Submitted to *Nature Computational Science*. (LA-UR-22-30360)

Kulichenko, M., N. E. Lubbers, J. Smith, Y. W. Li, R. A. Messerly, S. Tretiak, K. M. Barros and B. T. Nebgen. Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials.. Submitted to *Nature Computational Science*. (LA-UR-22-29407)

Sifain, A. E., L. Lystrom, R. A. Messerly, J. S. Smith, B. Nebgen, K. Barros, S. Tretiak, N. Lubbers and B. J. Gifford. Predicting phosphorescence energies and inferring wavefunction localization with machine learning. 2021. *Chemical Science*. **12** (30): 10207-10217. (LA-UR-21-21632 DOI: 10.1039/D1SC02136B)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, H. A. Nam, T. C. Germann, S. J. Fensin and K. M. Barros. Automated discovery of a robust interatomic potential for aluminum. Submitted to *Nature Communications*. (LA-UR-20-22194)

Smith, J. S., C. Devereux, K. K. Davis, R. Zubatyuk, K. M. Barros, O. Isayev and A. E. Roitberg. Extending the applicability of the ANI deep learning molecular potential to Sulfur and Halogens. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-20841)

Smith, J. S., M. A. Chigaev, K. M. Barros and N. E. Lubbers. Incorporating tensor information in Atomistic Convolutional Neural Networks. Submitted to *Journal of Chemical Physics*. (LA-UR-22-24861)

Smith, J. S., N. E. Lubbers, A. P. Thompson and K. M. Barros. Simple and efficient algorithms for training machine learning potentials to force data. Submitted to *Journal of Chemical Physics*. (LA-UR-20-24120)

Wu, X., S. Wen, H. Song, T. Frauenheim, S. Tretiak, C. Yam and Y. Zhang. Nonadiabatic Molecular Dynamics Simulations Based on Time-Dependent Density Functional Tight-Binding Method. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-32095)

Zhang, S., M. Z. Makos, R. B. Jadrich, E. Kraka, K. M. Barros, B. T. Nebgen, S. Tretiak, O. Isayev, N. E. Lubbers, R. A. Messerly and J. S. Smith. Discovering chemistry with the machine learning nanoreactor. Submitted to *Nature*. (LA-UR-22-29366)

Presentation Slides

Barros, K. M. Discovering Robust Inter-Atomic Potentials with Active Learning. Presented at *Telluride workshop*, Los Alamos, New Mexico, United States, 2020-07-28 - 2020-07-28. (LA-UR-20-25626)

Barros, K. M. Discovering Robust Inter-Atomic Potentials with Active Learning. Presented at *Southern California Hub Workshop*, Irvine, California, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28294)

Barros, K. M. Using machine learning to build robust interatomic potentials for bulk metals. Presented at *Machine Learning in Chemical and Materials Sciences*, Los Alamos, New Mexico, United States, 2021-05-13 - 2021-05-13. (LA-UR-21-24661)

Barros, K. M., S. J. Fensin, B. T. Nebgen, J. S. Smith, N. E. Lubbers, S. Tretiak, T. C. Germann and N. Mathew. Building surrogate models for interatomic potentials. Presented at *Simulations and computations of multiscale and out of equilibrium phenomena*, Los Alamos, New Mexico, United States, 2022-03-09 - 2022-03-10. (LA-UR-22-22233)

Barros, K. M. and J. S. Smith. Midterm LDRD Appraisal 20200209ER. . (LA-UR-20-29553)

Chigaev, M. A., J. S. Smith, K. M. Barros and N. E. Lubbers. Lightweight and Effective Tensor Sensitivity for Atomistic Neural Networks. . (LA-UR-22-28123)

Dahlbom, D. A., K. M. Barros and Y. W. Li. Fast Langevin Spin Dynamics on Many GPUs. . (LA-UR-21-27534)

Han, B. and K. M. Barros. Toward Atomistic Water Modules with Long-range Coulomb Interactions. . (LA-UR-22-27721)

Kulichenko, M., J. S. Smith, K. M. Barros and S. Tretiak. Diversification of ML datasets via “uncertainty” as a bias potential. Presented at *American Chemical Socienty Spring 2021*, Logan, Utah, United States, 2021-04-05 - 2021-04-30. (LA-UR-21-23523)

Makos, M. Z., R. B. Jadrich, E. Kraka, K. M. Barros, N. E. Lubbers and J. S. Smith. ML-based nano-reactor potential via active learning. Presented at *PASC21 Conference*, Geneva, Switzerland, 2021-07-05 - 2021-07-09. (LA-UR-21-26201)

Matin, S., M. S. Wilson, X. Bai, K. M. Barros, Y. W. Li, C. Miles, D. Brooks, M. Mourigal, C. D. Batista, H. Zhang and D. A. Dahlbom. Efficient Inference of Hamiltonian Parameters using Bayesian Optimization. Presented at *CSP Workshop, University of Georgia*, Online, New Mexico, United States, 2022-02-21 - 2022-02-21. (LA-UR-22-21827)

Matin, S. and K. M. Barros. Machine Learning Potentials with Long-Range Coulomb Interactions. Presented at *Arizona Days Workshop*, Los Alamos, New Mexico, United States, 2022-08-15 - 2022-08-16. (LA-UR-22-28586)

Sattar, N. S. and Y. W. Li. Accelerating parallel Monte Carlo simulations for statistical physics: Portability on many-core processors. Presented at *Parallel Computing Summer Research Internship Student Presentation*, Los Alamos, New Mexico, United States, 2021-08-05 - 2021-08-05. (LA-UR-21-27479)

Smith, J. S. Robust atomistic potentials from machine learning. . (LA-UR-21-23605)

Smith, J. S., K. M. Barros, S. Tretiak, N. Mathew, B. T. Nebgen, J. Chen, S. J. Fensin, T. C. Germann and N. E. Lubbers. Automated discovery of a robust interatomic potential for aluminum. Presented at *Arizona Days*, Pheonix, Arizona, United States, 2020-05-19 - 2020-05-19. (LA-UR-20-23703)

Smith, J. S., S. Tretiak, K. M. Barros, B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, S. J. Fensin, T. C. Germann, O. Isayev, A. E. Roitberg and R. Zubatyuk. Robust atomistic potentials from machine learning. . (LA-UR-19-31336)

Zhang, S. and R. A. Messerly. Nanoreactor: Discovering chemistry with machine learning. Presented at *2022 Theoretical Division Lightning Talk Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-10 - 2022-08-10. (LA-UR-22-28295)

Other

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, H. A. Nam, T. C. Germann, S. J. Fensin and K. M. Barros. Training dataset and model parameters for: "Automated discovery of a robust interatomic potential for aluminum". Dataset. (LA-UR-20-27198)

Zhang, S., B. T. Nebgen, N. E. Lubbers, R. A. Messerly and J. S. Smith. Dataset of energies and forces on nanoreactor for machine learned interatomic potentials. Dataset. (LA-UR-22-29658)

**Peer-reviewed*

Unlocking the Power of Tensor Cores with Mixed Precision Algorithms

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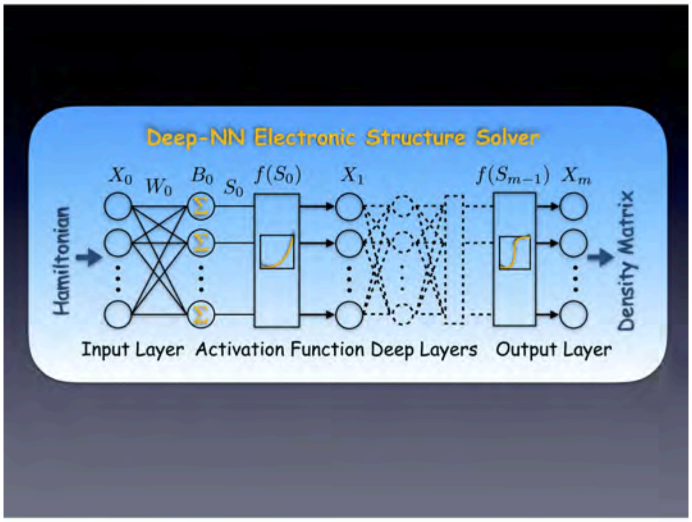
20200225ER



A schematic illustration of how the electornic structure problem can be mapped onto a deep neural network that naturally can take advantage of the computational structure of tensor cores.

Project Description

The world's most powerful computer, Summit at Oak Ridge National Laboratory, is currently rated at 144 petaflops, but it would exceed 4 exaflops only with its tensor core units if they only could be fully utilized for some general science application. This is currently not the case, since the tensor cores are highly specialized with a peak performance optimized for machine learning with convolutional deep neural networks using half-precision floating point operations. The goal of this project is the development of mixed precision algorithms that can harness the unprecedented power of tensor cores for more general real-world science applications, including electronic structure calculations and quantum-based molecular dynamics simulations. This would potentially extend accessible, predictive, simulation capabilities in time or length scale of materials systems by up to two-orders of magnitude compared to current methods. Our project will help maintain United States leadership in advanced scientific computing and directly support ongoing exascale research projects.

Technical Outcomes

This project has pioneered the field of quantum chemistry using hardware specialized for artificial intelligence applications. Our team has taking the lead in a rapidly evolving area of research. Novel algorithms and solvers within a multi-disciplinary coordinated design approach were successfully applied to overcome computational hurdles and limitations. Exceptional performance was demonstrated using tensor cores for electronic structure calculations, quantum-mechanical molecular dynamics simulations, and quantum response calculations.

Publications

*Peer-reviewed

Journal Articles

*Finkelstein, J. D., E. H. Rubensson, S. M. Mniszewski, C. F. A. Negre and A. M. Niklasson. Quantum Perturbation Theory Using Tensor Cores and a Deep Neural Network. 2022. *Journal of Chemical Theory and Computation*. **18** (7): 4255-4268. (LA-UR-22-21647 DOI: 10.1021/acs.jctc.2c00274)

Finkelstein, J. D., J. S. Smith, S. M. Mniszewski, K. M. Barros, C. F. A. Negre, E. H. Rubensson and A. M. Niklasson. Mixed Precision Fermi-Operator Expansion on Tensor Cores from a Machine Learning Perspective. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-20350)

*Finkelstein, J., J. S. Smith, S. M. Mniszewski, K. Barros, C. F. A. Negre, E. H. Rubensson and A. M. N. Niklasson. Quantum-Based Molecular Dynamics Simulations Using Tensor Cores. 2021. *Journal of Chemical Theory and Computation*. **17** (10): 6180-6192. (LA-UR-21-25427 DOI: 10.1021/acs.jctc.1c00726)

Presentation Slides

Finkelstein, J. D. Quantum-based Molecular Dynamics with Tensor Cores. . (LA-UR-21-25428)

Finkelstein, J. D. Quantum-based molecular dynamics simulations using Tensor cores. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, San Diego, California, United States, 2022-03-26 - 2022-03-30. (LA-UR-22-29326)

Finkelstein, J. D. Using Tensor Cores for Electronic Structure Calculations and Molecular Dynamics. Presented at *Presentation at Lawrence Berkeley Lab (virtual)*, Berkeley, California, United States, 2022-01-12 - 2022-01-12. (LA-UR-22-29328)

Niklasson, A. M. Unlocking the Power of Tensor Cores with Mixed Precision Algorithms. Presented at *Informal zoom meeting with google sandbox team*, Los Alamos, New Mexico, United States, 2021-04-26 - 2021-04-26. (LA-UR-21-23932)

Niklasson, A. M. Unlocking the Power of Tensor Cores with Mixed Precision Algorithms, LANL Project Overview. . (LA-UR-22-22232)

Niklasson, A. M. Quantum-based Molecular Dynamics using Deep Neural Networks and AI Hardware. Presented at *TSRC Teluuride Workshop*, Telluride, Colorado, United States, 2022-07-11 - 2022-07-11. (LA-UR-22-24840)

Niklasson, A. M., J. D. Finkelstein and C. F. A. Negre. Quantum-based Molecular Dynamics using Deep Neural Networks and AI Hardware. Presented at *ACS fall meeting in Chicago*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-21. (LA-UR-22-29596)

Dielectric Antenna Array for Pinpoint Data/Energy Targeting

John Singleton
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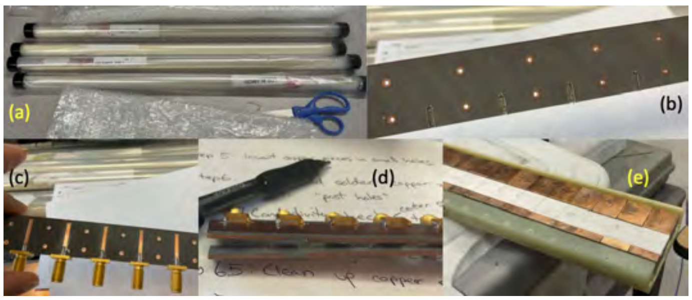


The project aims to design, construct, and test a transmitter based on dielectric antennas that is capable of focusing a signal at a precise point. Close to this point the signal would be easily understood or decoded; at all other locations the signal would be scrambled. The images show the CAD/CAM components for monolithic antenna array. (a) CNC machined G10 and alumina components on arrival. (b) Detail of CNC milled slots and copper plating on antenna base. (c) Monolithic second layer with signal input plugs. (d) Antenna layers prior to bonding. (e) Comparison view of non-monolithic prototype used in year 1 of project comprising many more machined parts and more complex assembly.

Project Description

This project designs, constructs and tests a new type of radio transmitter that focuses a signal so that it is easily understood at an intended target but scrambled in other places. The transmitter comprises an array of special dielectric antennas developed at Los Alamos National Laboratory. In these antennas, the emission of radio waves is due to moving polarization currents that travel faster than the speed of light in a vacuum, and which are distributed throughout the whole dielectric. These antennas can be built in unusual shapes (flat panels, cylinders, disks), optimized to particular situations and could form part of the ceramic armor applied to future armored vehicles. The outcome represents a fundamental shift in wireless battlefield communications. For over a hundred years procedures have hardly changed; signals are broadcast with little or no directivity, selectivity of reception being via the use of one or more narrow frequency bands. These methods are vulnerable to interception and jamming. In place of this, our technology employs a spread of frequencies to transmit information to a precise location. Decoding/jamming the signal elsewhere is much harder, especially in the context of a rapidly changing conflict situation where transmitter and target are moving.

Technical Outcomes

Dielectric antennas were used to transmit broadband signals that are reproduced in a comprehensible form only at a chosen position. An array of antennas was designed and constructed using computer numerical control machining of a small number of monolithic parts, providing considerable advantages in manufacturing, supply chain and size, weight and power compared to conventional antennas. The dielectric antennas were found to have excellent frequency bandwidth. These achievements resulted in a 2022 R&D 100 award.

Publications

Journal Articles

Schmidt, A. C. and J. Singleton. Fatal flaws in the theory of electromagnetic radiation that disobeys the inverse-square law: mathematical and physical considerations. Submitted to *Journal of Plasma Physics*. (LA-UR-20-23586)

Schmidt, A. C. and J. Singleton. Electromagnetic radiation from a polarization current in circular faster-than-light motion; theory and an experimentally realized example. Submitted to *Journal of Plasma Physics*. (LA-UR-21-30110)

*Singleton, J., A. C. Schmidt, C. Bailey, J. Wigger and F. Krawczyk. Information Carried by Electromagnetic Radiation Launched from Accelerated Polarization Currents. 2020. *Physical Review Applied*. **14** (6): 064046. (LA-UR-20-23902 DOI: 10.1103/PhysRevApplied.14.064046)

Singleton, J. and A. C. Schmidt. Launching information from faster-than-light polarization currents. Submitted to *Research Features*. (LA-UR-21-30356)

Books/Chapters

Singleton, J. Cyclotron resonance in metals. (LA-UR-22-26196)

Reports

Schmidt, A. C., J. Singleton and J. B. Warner. LightSlingers. Unpublished report. (LA-UR-22-23925)

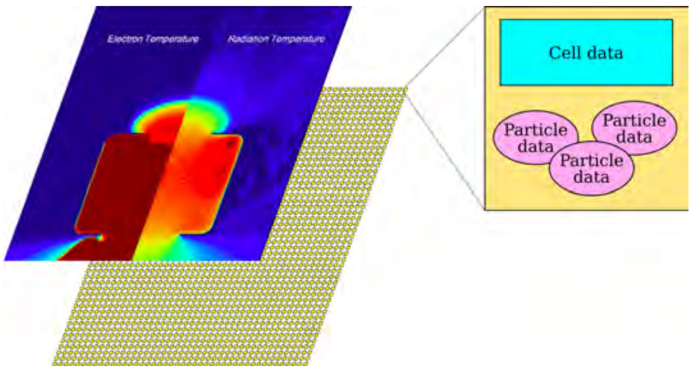
Presentation Slides

Schmidt, A. C. and J. Singleton. Meet the Lightslingers. . (LA-UR-22-20640)

**Peer-reviewed*

Monte Carlo Transport Simulations on a Billion-Core Approximate-Computing Platform

Alex Long
20210849ER



Mapping of an Implicit Monte Carlo (IMC) particle simulation onto prototype hardware produced by Singular Computing. Each yellow square represents a single compute core, called an approximate processing element (APE). Only a single chip, with 2,112 APEs, is illustrated. The existing prototype board contains 33,792 APEs, and the final hardware is targeting over a billion. This LDRD project seeks to simulate particle movement, reflection, and absorption across varying material temperatures and opacities on hardware offering tremendous peak performance and energy efficiency but that is highly challenging to program due to locality and numerical-precision constraints.

Project Description

Through this project we will explore a different type of computer that is faster and uses less power but it has some imprecise arithmetic. If we can adapt an important physics algorithm to work well on this new computer we have a chance to greatly improve the workflows of users in the National Nuclear Security Administration (NNSA).

Technical Outcomes

This project succeeded in developing the tools and algorithmic adaptations needed to develop simulation codes for this novel, imprecise computer. Imprecise arithmetic and limited functionality required the team to implement novel solutions compared to standard physics and computer science algorithms. This project has laid the foundation for implementing a physics algorithm on this new novel computer architecture and gives Los Alamos National Laboratory a chance to lead in this unique computer architectural space.

Publications

Presentation Slides

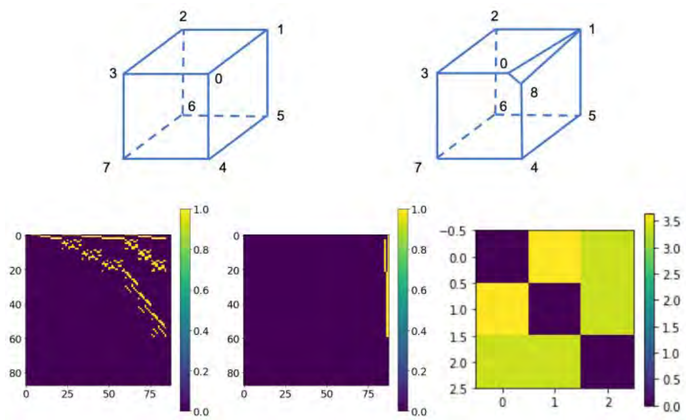
Long, A. R. An Overview of the Implicit Monte Carlo Algorithm. . (LA-UR-21-23650)

Pakin, S. D. Computing Logarithms on S1 Hardware. . (LA-UR-22-21367)

**Peer-reviewed*

Shape Matching of 3-Dimensional Computer-Aided Design (CAD) Models in Automatic Hexahedral Meshing Workflows

Rao Garimella
20210906ER



Evaluation of the RESCAL Tensor Factorization software to evaluate similarity between two identical cubes (top left) and one "dirty" cube (top right). The bottom left and bottom middle images show the two slices of the tensor and the bottom right shows the similarity metric between the cubes. This simple example shows success with shape matching using Relational Tensor Factorization

Project Description

Many national security applications, including performance assessments of nuclear and conventional weapons systems, involve complex multiphysics simulations. These simulations require the domain (or geometric model) to be tiled with simpler shapes called hexahedral elements to form a computational mesh Generating these meshes is at best a semi-automatic process guided by experienced analysts and can take up as much 50% of the design-analysis cycle time. Our research will apply machine learning techniques to match input geometries to models that the system already knows how to decompose and mesh. This project will serve as proof of principle that such shape matching is possible without huge training data sets. In the short term, we expect to be able to identify "dirty geometry" (unexpected hidden geometric modeling artifacts) that trip up engineers trying to mesh the models. The long term plan of using machine learning for hexahedral meshing holds the promise of capturing the intuition of experienced engineers by "learning" general strategies for meshing such models. This will eventually have far-ranging impacts in many Department of Energy (DOE) applications with national security implications, including weapons system performance, seismic monitoring for non-proliferation, nuclear energy production and others.

Technical Outcomes

This project explored the viability of several shape matching algorithms as applied to 3-dimensional (3D) computer aided design models, identifying their particular strengths and highlighting the need for further research. The team concluded that while it is possible to perform shape matching of 3D shapes using limited training data (hundreds to thousands of models, not millions), particular techniques explored lack the sophistication to match shapes with the necessary fidelity to use in meshing pipelines.

Publications

Conference Papers

Garimella, R. V., C. Garcia Cardona and N. Ray. AI for Automatic Hexahedral Meshing. Presented at *AI@DOE (https://www.orau.gov/AI-DOERoundtable)*. (Virtual, New Mexico, United States, 2021-12-01 - 2021-12-01). (LA-UR-21-31688)

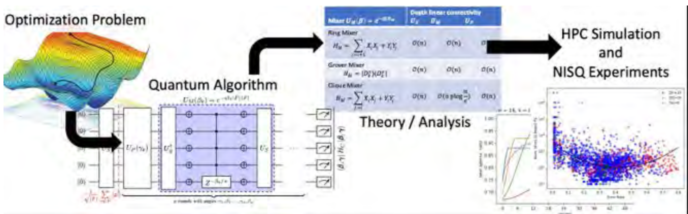
Reports

Payne, E. R., N. Ray, R. V. Garimella and C. Garcia Cardona. Shape Matching for Hexahedral Mesh Generation. Unpublished report. (LA-UR-21-28999)

**Peer-reviewed*

Application-Specific Hamiltonian Simulation Methods

Stephan Eidenbenz
20220656ER



The nature of quantum algorithms and quantum computers requires a thorough design of novel quantum algorithms for mission-relevant optimization problems, such as network partitioning or solveing Hubbard models. Theoretical performance analysis coupled with numerical experiments and experiments on Noisy Intermediate Scale Quantum (NISQ) devices will allow us to assess the near- and long-term impacts of our algorithms

Project Description

Our grand vision is to close the gap between powerful quantum algorithms, which provide asymptotic speed-ups over classical algorithms, and their actual suitability for Los Alamos National Laboratory mission-relevant computational problems. The nature of this gap is as follows: quantum algorithms are known for broad classes of computational problems, but almost no work has been done to formulate mission-relevant computational problems in terms of these quantum meta-algorithms (with modifications as needed) to determine actual resource requirements of a quantum computing device required to execute such computations. In other words: If a large (say 1 million qubits) fault-tolerant quantum computer suddenly appeared, we would presently not know if we could use it for most, if not all, mission-relevant computational problems. The reason is that we do not yet know the actual quantum resources needed for these problems as we have not designed the detailed algorithms for it. We aim to close this gap for two specific problems: 1. Network partitioning optimization 2. Superconductivity studies of correlated materials with the fermionic Hubbard model using direct quantum simulation.

Technical Outcomes

The project team developed Hamiltonian simulation techniques that focus on Hamiltonians as they arise in Quantum Alternating Operator Ansatz algorithms for classical optimization problems. The team developed novel mixer operators for several constrained optimization problems, including Densest k-Subgraph. Dicke state construction is an important building block of these algorithms, for which the team found an improved lower bound. Corresponding numerical simulation as well as actual experiments on quantum hardware complemented the outcomes of the project.

Publications

Journal Articles

Golden, J. K., A. Baertschi, D. O'Malley and S. J. Eidenbenz. The Quantum Alternating Operator Ansatz for Satisfiability Problems. Submitted to *Quantum*. (LA-UR-23-20702)

Golden, J. K., D. O'Malley, S. J. Eidenbenz and A. Baertschi. QAOA Mixer Comparison and Experimental Quantum Advantage for Constrained Optimization Problems. Submitted to *Physical Review Letters*. (LA-UR-22-20645)

Golden, J. K., D. O'Malley and H. S. Viswanathan. Quantum Preconditioners and Hydrological Linear Systems. Submitted to *Nature Computational Science*. (LA-UR-22-24431)

R. Pelofske, E. A. Mapping state transition susceptibility in reverse annealing. Submitted to *Physical review research*. (LA-UR-22-31301)

R. Pelofske, E. A. Comparing Three Generations of D-Wave Quantum Annealers for Minor Embedded Combinatorial Optimization Problems. Submitted to *IEEE Transactions on Quantum Engineering*. (LA-UR-23-20101)

R. Pelofske, E. A. 4-clique network minor embedding for quantum annealers. Submitted to *IOP Quantum Science and Technology*. (LA-UR-23-20504)

R. Pelofske, E. A. Analysis of a Programmable Quantum Annealer as a Random Number Generator. Submitted to *New Journal of Physics*. (LA-UR-23-23112)

R. Pelofske, E. A., A. Baertschi and S. J. Eidenbenz. Short-Depth QAOA circuits and Quantum Annealing on Higher-Order Ising Models. Submitted to *Quantum*. (LA-UR-23-22023)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Noise Dynamics of Quantum Annealers: Estimating the Effective Noise Using Idle Qubits. Submitted to *Quantum Science and Technology - IOPscience*. (LA-UR-22-27371)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Initial state encoding via reverse quantum annealing and h-gain features. Submitted to *IEEE Transactions on Quantum Engineering*. (LA-UR-23-22902)

R. Pelofske, E. A., H. N. Djidjev and G. Hahn. Solving Larger Optimization Problems Using Parallel Quantum Annealing. Submitted to *Quantum Information Processing*. (LA-UR-22-24790)

*Pelofske, E., A. Bartschi and S. Eidenbenz. Quantum Volume in Practice: What Users Can Expect From NISQ Devices. 2022. *IEEE Transactions on Quantum Engineering*. **3**: 3102119. (LA-UR-22-22058 DOI: 10.1109/TQE.2022.3184764)

*Pelofske, E., G. Hahn, D. O'Malley, H. N. Djidjev and B. S. Alexandrov. Quantum annealing algorithms for Boolean tensor networks. 2022. *Scientific Reports*. **12** (1): 8539. (LA-UR-21-27414 DOI: 10.1038/s41598-022-12611-9)

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R. Pelofske, E. A., A. Baertschi, B. Garcia, B. Kiefer and S. J. Eidenbenz. Quantum Telecloning on NISQ Computers. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Broomfield, Colorado, United States, 2022-09-18 - 2022-09-23). (LA-UR-22-23967)

R. Pelofske, E. A., A. Baertschi and S. J. Eidenbenz. Quantum Annealing vs. QAOA: 127 Qubit Higher-Order Ising Problems on NISQ Computers. Presented at *isc hpc 2023*. (Hamburg, Germany, 2023-05-21 - 2022-12-25). (LA-UR-22-33077)

Reports

Aktar, S., A. Baertschi, A. Badawy and S. J. Eidenbenz. Scalable Experimental Bounds for Entangled Quantum State Fidelities. Unpublished report. (LA-UR-22-30105)

Presentation Slides

Baertschi, A. QAOA for Hamming weight constrained problems. Presented at *Workshop on Quantum Algorithms for Financial Applications (IEEE Quantum Week)*, Broomfield, Colorado, United States, 2022-09-23 - 2022-09-23. (LA-UR-22-30368)

Baertschi, A. and S. J. Eidenbenz. Short-Depth Circuits for Dicke State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Broomfield, Colorado, United States, 2022-09-19 - 2022-09-23. (LA-UR-22-30140)

R. Pelofske, E. A., A. Baertschi and S. J. Eidenbenz. Quantum Annealing vs. QAOA: 127 Qubit Higher-Order Ising Problems on NISQ Computers. Presented at *International Network on Quantum Annealing*, Virtual, New Mexico, United States, 2023-02-28 - 2023-02-28. (LA-UR-23-21928)

Posters

Golden, J. K., A. Baertschi, S. J. Eidenbenz and D. O'Malley. Numerical evidence for exponential speed-up of QAOA over unstructured search for approximate constrained optimization. Presented at *Southwest Quantum Information and Technology*, Berkeley, California, United States, 2022-10-20 - 2022-10-22. (LA-UR-22-31458)

Other

R. Pelofske, E. A. Dataset for 4-clique network minor embedding for quantum annealers. Dataset. (LA-UR-23-20505)

R. Pelofske, E. A. Dataset for Mapping state transition susceptibility in reverse annealing. Dataset. (LA-UR-23-21780)

R. Pelofske, E. A., A. Baertschi and S. J. Eidenbenz. Dataset for Quantum Annealing vs. QAOA: 127 Qubit Higher-Order Ising Problems on NISQ Computers. Dataset. (LA-UR-23-21597)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Dataset for Noise Dynamics of Quantum Annealers: Estimating the Effective Noise Using Idle Qubits. Dataset. (LA-UR-23-21598)

**Peer-reviewed*

Settingless Microgrid Protection

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Dynamic State Estimation (DSE) based protection can help increase the size of microgrids by allowing for protection coordination, even with inverter-interfaced microgrids and a relatively small number of protective devices. A proposed microgrid for a community college campus and nearby community loads is illustrated.

Project Description

Inverter-interfaced microgrids – in which both renewable (such as photovoltaic-solar and hydro generators) and conventional (such as diesel and natural gas prime movers) energy sources are employed – have potential to incorporate large and complex areas for both grid-connected and islanded operation. Proper protection, however, remains a pressing technical challenge preventing their widespread application. Novel protection methods could provide benefits. Coupling fossil-fueled generation or co-generation via an inverter may eliminate fault currents and help improve dynamic stability of microgrids. Practical inverter-interfaced microgrid deployments are unable to make use of protection coordination to reduce outage areas during faults, limiting their size; adequate protection may therefore enable larger microgrids that span sizable, dispersed facilities – such as military bases or Los Alamos National Laboratory itself – or remote communities, ultimately increasing resilience of the bulk power system. The proposed Dynamic State Estimation (DSE) algorithm promotes protection of inverter-interfaced microgrids and aids their safe operation. Existing work on DSE focuses on protection on elements with parameters known in advance (e.g., overhead lines, transformers) with minor unknown quantities (e.g., fault location); this proposed work extends DSE to portions of the network with loads, which have a far greater degree of uncertainty in their parameters.

Technical Outcomes

Dynamic models for downstream aggregated loads were developed; including simplified models of three-phase resistive-inductive loads and a model of a three-phase induction motor. For implementation, an “orchestrator” program was developed for selecting among multiple models.; it spawns multiple Dynamic State Estimation (DSE) executable child processes, where each process implements DSE for a particular model. The DSE executables receive measured states from the “orchestrator” and respond with estimated state values and an estimation confidence value.

Publications

Conference Papers

Barnes, A. K., A. Mate, J. M. V. Bikorimana and R. J. Castillo. Dynamic State Estimation for Load Bus Protection on Inverter-Interfaced Microgrids. Presented at *IEEE PES & IAS PowerAfrica Conference 2022*. (Kigali, Rwanda, 2022-08-22 - 2022-08-26). (LA-UR-22-22686)

Barnes, A. K., S. Basu and A. Mate. Dynamic State Estimation-Based Protection for Induction Motor Loads. Presented at *IEEE/PES 54th North American Power Symposium*. (Salt Lake City, Utah, United States, 2022-10-09 - 2022-10-11). (LA-UR-22-27020)

Presentation Slides

Barnes, A. K., A. Mate, J. Bikorimana and R. Castillo. Dynamic State Estimation for Load Bus Protection on Inverter-Interfaced Microgrids. Presented at *PowerAfrica 2022*, Kigali, Rwanda, 2022-08-22 - 2022-08-26. (LA-UR-22-28716)

Barnes, A. K., S. Basu and A. Mate. Dynamic State Estimation-Based Protection for Induction Motor Loads. Presented at *North American Power Symposium*, Salt Lake City, Utah, United States, 2022-10-09 - 2022-10-11. (LA-UR-22-30190)

Posters

Basu, S., A. K. Barnes and A. Mate. Dynamic State Estimation-Based Protection for Induction Motor Loads. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27074)

**Peer-reviewed*

Quantum Information-Based Complexity

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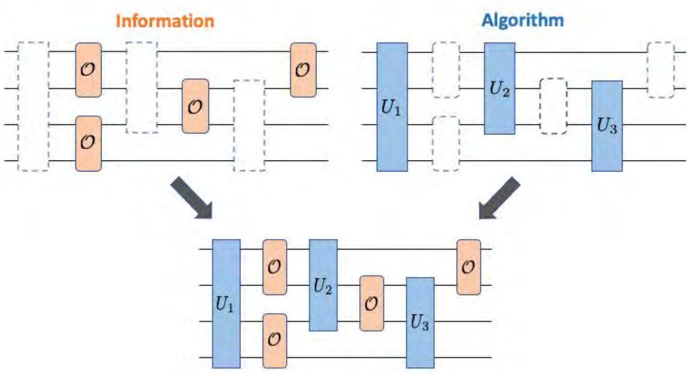

Information-based complexity (IBC) provides powerful tools to analyze the computational complexity of continuous problems in the classical setting. Key to IBC is the separation between the information about the problem instance and the algorithm that transforms this information into a solution. Such a separation does not occur naturally in the quantum setting, where algorithm and information are intertwined. Here the team interprets a quantum query algorithm (top right) as a supermap that transforms quantum operations, i.e. information in the form of queries, (top left) into another quantum operation that solves the problem (bottom).

Project Description

Developing simulation capabilities and deploying computing platforms to analyze and predict the performance, safety, and reliability of nuclear weapons became essential since physical nuclear tests have been banned. Given the extraordinary complexity of nuclear weapons systems there is a need for very large scale modeling and simulation and the computational resources grow exponentially. A similar problem is encountered when studying quantum matter; even the simulation of microscopic molecules can be beyond the reach of supercomputers. Quantum computers promise to solve some problems more efficiently than any classical computer can. Unfortunately, identifying such problems has proven hard and a quantum speed up has been shown only for a small number of problems. In this project we will develop a theoretical framework that will enable us to analyze the quantum complexity of problems and develop efficient algorithms for solving them. In particular, our proposed formalism and tools will help rule out problems with no possibility of quantum advantage. By doing so, they will guide research efforts towards fruitful directions.

Publications

Journal Articles

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O'Malley, D., J. K. Golden, Y. Subasi, R. B. Lowrie and S. J. Eidenbenz. A near-term quantum algorithm for solving linear systems of equations based on the Woodbury identity. Submitted to *Quantum*. (LA-UR-22-23447)

Volkoff, T. J. and Y. Suba\xc5\x9f\xc4\xb1. Ancilla-free continuous-variable SWAP test. 2022. *Quantum*. **6**: 800. (LA-UR-22-21141 DOI: 10.22331/q-2022-09-08-800)

Presentation Slides

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Schoute, E., M. Beverland and V. Kliuchnikov. Surface code compilation via edge-disjoint paths. Presented at *Quantum Science Center*, College Park, Maryland, United States, 2022-02-02 - 2022-02-02. (LA-UR-22-20684)

Posters

Beverland, M., V. Kliuchnikov and E. Schoute. Surface code compilation via edge-disjoint paths. Presented at *Quantum Information Processing 2022*, Pasadena, California, United States, 2022-03-07 - 2022-03-07. (LA-UR-22-21915)

**Peer-reviewed*

Accelerated Monte Carlo Algorithms without Detailed Balance

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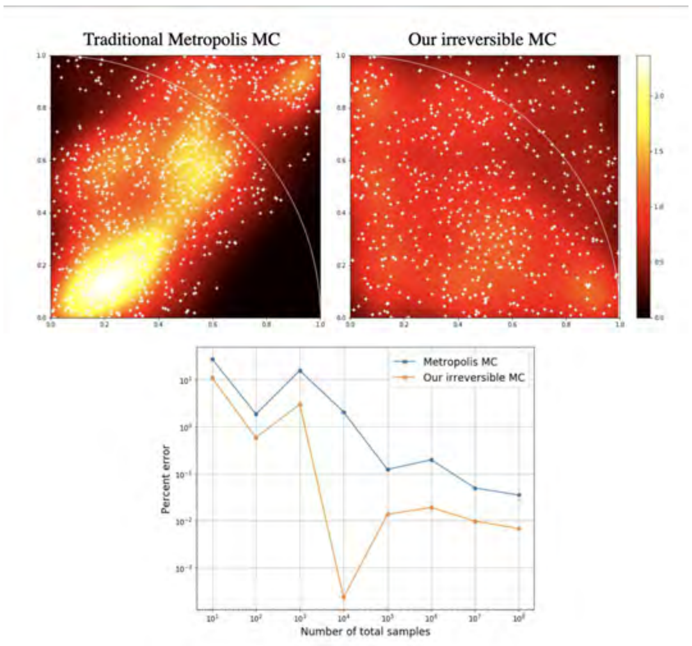

Getting good random samples according to a distribution can be a challenging task especially in high dimensions. Efficient Monte Carlo algorithms developed based on irreversibility can alleviate this problem by suppressing the diffusion behavior of random walks. In the example of sampling from a uniform distribution shown here, the irreversible method developed through LDRD support generates a much more uniform distribution, resulting in higher accuracy and better statistics compared to the traditional Metropolis Monte Carlo method given the same number of total samples.

Project Description

The project will develop smart, efficient, and parallel stochastic methods for computer simulations that are readily scalable on leadership-class supercomputers. The Monte Carlo (MC) algorithms to be developed in this work are a fundamental tool in computational physics that has a tremendous range of mission-relevant applications across Los Alamos National Laboratory (LANL), National Nuclear Security Administration (NNSA), and Department of Energy (DOE). MC enables the study of neutron and radiation transport and defect dynamics in materials at the mesoscale, making MC methods the workhorses for studying nuclear physics, high energy physics, matter phases, transitions, and aging, as well as equilibrium and non-equilibrium phenomena. Improved MC methods can greatly benefit scientific machine learning, uncertainty quantification, and emulation of quantum computers. General improvements to MC methodology proposed in this work could greatly benefit all of these fields. Moreover, MC methods are naturally suitable for advanced parallel computer hardware such as many-core processors and graphics processing unit (GPU) accelerators, so successful execution of this work will reduce the time-to-solution for solving scientific grand challenges on the DOE's leadership-class supercomputers.

Publications

Journal Articles

Casiano Diaz, E., C. M. Herdman and A. Del Maestro. PIGSFLI: A Path-Integral Ground State Monte Carlo Algorithm for Entanglement of Lattice Bosons. Submitted to *SciPost Physics*. (LA-UR-22-26315)

Casiano Diaz, E., K. M. Barros, Y. W. Li and A. Del Maestro. Reduction of Autocorrelation Times in Lattice Path Integral Quantum Monte Carlo via Direct Sampling of the Truncated Exponential Distribution. Submitted to *Computer Physics Communications*. (LA-UR-23-21469)

*Ferreira, T., S. R. Acharya, Y. W. Li, D. S. Parker, A. S. Sefat and V. R. Cooper. Unintended consequence of topochemical reduction of SrFeO3 to SrFeO2: Design of infinite layered oxides. 2021. *Physical Review Materials*. **5** (12): 123401. (LA-UR-21-27840 DOI: 10.1103/PhysRevMaterials.5.123401)

Conference Papers

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Presentation Slides

Li, Y. W. Machine Learning Assisted Simulations of Materials Thermodynamics. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-28 - 2022-03-03. (LA-UR-22-21946)

Li, Y. W. and T. Vogel. Accelerating Multicanonical Sampling with Irreversibility. Presented at *35th Annual CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens (Virtual), Georgia, United States, 2022-02-21 - 2022-02-24. (LA-UR-22-22032)

Wilson, M. S., K. M. Barros, Y. W. Li, S. Matin, X. Bai, C. Miles, C. Batista and M. Mourigal. Fitting Hamiltonian Parameters with Bayesian Optimization of Numerical Simulations. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22669)

Wilson, M. S., X. Bai, Y. W. Li, K. M. Barros, C. Batista and M. Mourigal. Revealing the Rich Magnetic Behaviors of FeI2 with Monte Carlo Simulation. Presented at *33rd IUPAP Conference on Computational Physics*, Austin, Texas, United States, 2022-08-01 - 2022-08-04. (LA-UR-22-27850)

Wilson, M. S., Y. W. Li, K. M. Barros, C. Batista, M. Mourigal and X. Bai. Examining the Rich Magnetic Phases of FeI2 with Monte Carlo Simulation. Presented at *36th Annual CSP Workshop*, Athens, Georgia, United States, 2023-02-20 - 2023-02-24. (LA-UR-23-21888)

Posters

Sattar, N. S. and Y. W. Li. Accelerating Parallel Monte Carlo Simulations for Statistical Physics: Portability on Many-Core Processors. Presented at *Supercomputing 21*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-19. (LA-UR-21-28319)

**Peer-reviewed*

Statistical Learning for Field Theories

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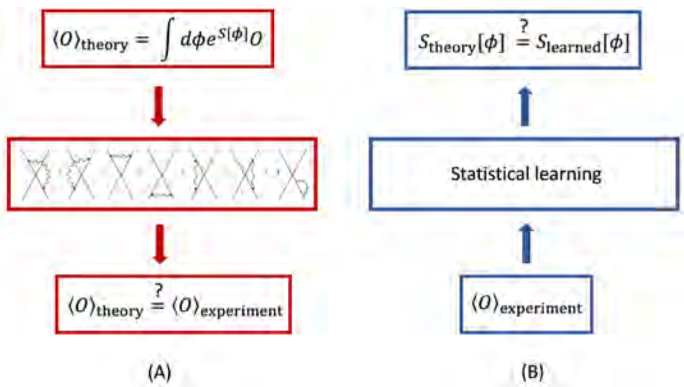

A traditional way to validate a conjectured field theory consists in performing hard computations of some observables, and then comparing them with experiment or expensive lattice simulations (A). This project develops a novel approach to validating field theories based on statistical learning, where experimental or simulation data are used to learn the model and comparing it to the theoretical one (B), which has a potential benefit of computational tractability.

Project Description

Field theories lie at the heart of modern natural sciences, with a wide range of interdisciplinary applications ranging from classical electrodynamics or gravitation, through statistical physics or turbulent flows, to condensed matter or high energy physics. Non-linearities of interactions in non-trivial field theories typically preclude analytic precise predictions within these models even when the underlying physics is well understood. Radically new ideas for validating field theory models are required for making progress in non-linear science in the twenty-first century. The goals of this proposal are two-fold: first, development of novel methods for learning of field theories from scarce experimental measurements or data obtained from costly first-principles simulations; second, demonstration of our central hypothesis that even those field theories for which generation of quantitative predictions is intractable can be still be validated using a novel statistical-learning based method. If successful, the proposed research will likely produce a substantial impact on the modern theory of high-energy, condensed matter, and turbulence physics which are among the priority research directions for Los Alamos National Laboratory (LANL), leading to a new path towards non-perturbative methods in Quantum Field Theory and fluid dynamics and advancing the forefront of these fields.

Publications

Journal Articles

Jayakumar, A., M. D. Vuffray and A. Lokhov. Learning Energy Based Representations of Quantum Many-Body States. Submitted to *Nature Physics*. (LA-UR-23-23196)

Shastry, A., A. Jayakumar, C. Bhattacharyya and A. Patel. Reliable Quantum Kernel Classification using fewer Circuit Evaluations. Submitted to *Physical Review X*. (LA-UR-22-28394)

Tasseff, B. A., T. Albash, Z. A. Morrell, M. D. Vuffray, A. Lokhov, S. Misra and C. J. Coffrin. On the Emerging Potential of Quantum Annealing Hardware for Combinatorial Optimization. Submitted to *Operations Research*. (LA-UR-22-29705)

Vuffray, M., C. Coffrin, Y. A. Kharkov and A. Y. Lokhov. Programmable Quantum Annealers as Noisy Gibbs Samplers. 2022. *PRX Quantum*. **3** (2): 020317. (LA-UR-20-28047 DOI: https://doi.org/10.1103/PRXQuantum.3.020317)

Conference Papers

Jayakumar, A., M. D. Vuffray and A. Lokhov. Energy based models for tomography of quantum spin-lattice systems. Presented at *Machine Learning and the Physical Sciences*. (New Orleans, Louisiana, United States, 2022-12-03 - 2022-12-03). (LA-UR-22-30151)

Ren, C. X., S. Misra, M. D. Vuffray and A. Lokhov. Learning Continuous Exponential Families Beyond Gaussian. Presented at *NeurIPS 2022*. (New Orleans, Louisiana, United States, 2022-11-28 - 2022-11-28). (LA-UR-22-25979)

Reports

Morrell, Z. A., M. D. Vuffray, A. Lokhov, A. Baertschi, T. Albash and C. J. Coffrin. Signatures of Open and Noisy Quantum Systems in Single-Qubit Quantum Annealing. Unpublished report. (LA-UR-22-28691)

Presentation Slides

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Lokhov, A. Learning of classical lattice Hamiltonians. Presented at *Seminar at RPI*, Online, New Mexico, United States, 2021-10-27 - 2021-10-27. (LA-UR-21-30704)

Lokhov, A. On the emerging potential of quantum annealing hardware for combinatorial optimization. Presented at *INFORMS 2022*, Indianapolis, Indiana, United States, 2022-10-16 - 2022-10-19. (LA-UR-22-30902)

Lokhov, A. Learning continuous exponential families beyond Gaussian. Presented at *Information Theory and Applications Workshop*, San Diego, California, United States, 2023-02-12 - 2023-02-12. (LA-UR-23-21681)

Lokhov, A., D. Livescu and R. W. Bent. Physics Informed Machine Learning at LANL. . (LA-UR-22-28986)

Pang, Y., A. Jayakumar, E. McKinney, C. J. Coffrin, M. D. Vuffray and A. Lokhov. Unreasonable effectiveness of pairwise Markov random fields in finding ground states of stoquastic Hamiltonians. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22280)

Posters

Jayakumar, A., M. D. Vuffray and A. Lokhov. Energy based models for tomography of quantum spin-lattice systems. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*, New Orleans, Louisiana, United States, 2022-11-28 - 2022-12-03. (LA-UR-22-32410)

**Peer-reviewed*

Theory and Modeling of Polariton Chemistry for Quantum Information Science

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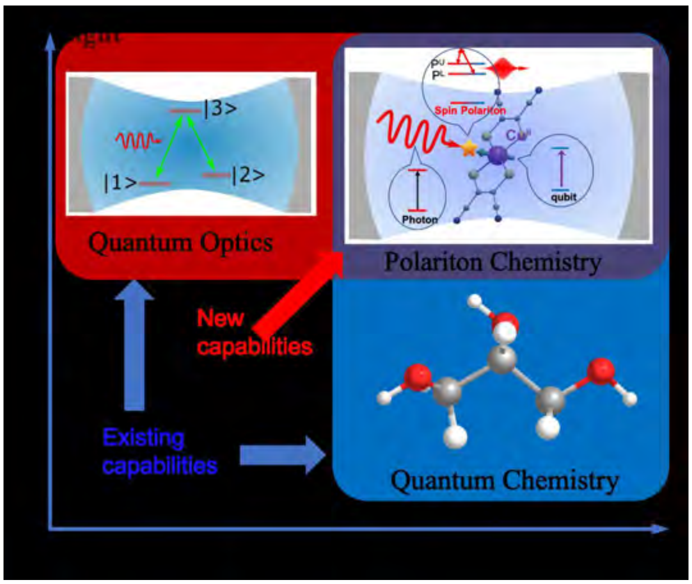
20220527ECR



Modeling of the polaritons (formed due to strong light-matter interaction) remains a big challenge. While current theories (quantum optics and quantum chemistry) are good at treating the light-matter interaction in separate domains by simplifying either light or matter, there is no reliable and computationally feasible ab initio framework that can describe the emergent properties of polaritons. This project will overcome the current theoretical gap and computational shortcoming. A new ab initio quantum many-body theory for polariton chemistry will be delivered, which will be used to study spin polariton mediated quantum information transduction.

Project Description

This project will develop quantum many-body theory for polariton chemistry where both matter and light are equally important. Such development will bridge two large subfields, namely the quantum chemistry and quantum optics, filling current theoretical and modeling gaps. This project will provide brand new modeling capabilities which is critical for understanding the strong light-matter interaction induced collective behaviors in materials. The developed modeling capabilities with have broad applications in many Los Alamos National Laboratory/Department of Energy mission-related areas, particularly benefits the Information Science and Technology Priority #1 Computational Multiphysics and the Materials for the Future Priority #1: Materials and Phenomena underpinning Quantum Information Science. This project will demonstrate its applications in quantum information science by studying the spin-polariton mediated quantum information transduction. Besides, the developed modeling tools can be used to advance modeling of photoactive materials and design new quantum materials. The high-level goals of the project are to develop a modeling capability to describe the collective behaviors in realistic materials and to apply the capability for the prediction, control and design of specific material properties for applications in quantum information science and energy innovation.

Publications

Journal Articles

Chamaki, D., N. Tkachenko, Y. Zhang, S. Tretiak, P. Dub and B. K. Kendrick. Non-adiabatic molecular dynamics on quantum computers. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-22-29519)

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Timmer, D., F. Zheng, M. Gittinger, T. Quenzel, D. C. L \xc3\xbcnemann, K. Winte, Y. Zhang, M. E. Madjet, A. L \xc3\xbctzen, J. Zhong, A. D. Sio, T. Frauenheim, S. Tretiak and C. Lienau. Charge Delocalization and Vibronic Couplings in Quadrupolar Squaraine Dyes. 2022. *Journal of the American Chemical Society*. (LA-UR-22-28452 DOI: 10.1021/jacs.2c08682)

*Wu, X., S. Wen, H. Song, T. Frauenheim, S. Tretiak, C. Yam and Y. Zhang. Nonadiabatic molecular dynamics simulations based on time-dependent density functional tight-binding method. 2022. *The Journal of Chemical Physics*. **157** (8): 84114. (LA-UR-21-32095 DOI: 10.1063/5.0100339)

Wu, X., S. Wen, T. Frauenheim, S. Tretiak, C. Yam and Y. Zhang. Dynamical Insights into Plasmon-Mediated Chemical Transformations. Submitted to *Journal of the American Chemical Society*. (LA-UR-22-27318)

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Reports

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Presentation Slides

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Zhang, Y. Quantum electronic structure theory and first-principles modeling of spin-phonon relaxation. Presented at *TSRC Workshop ``From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information"*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25417)

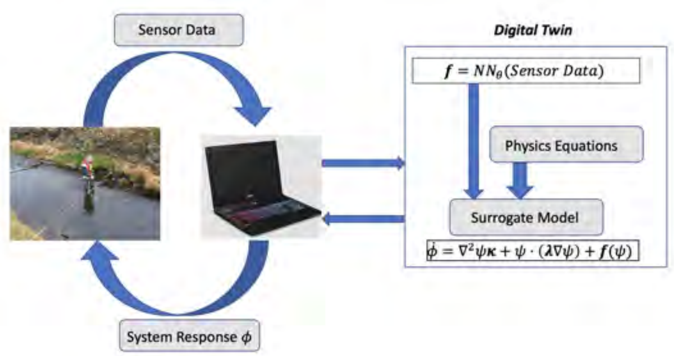
Zhang, Y. Non-adiabatic molecular dynamics in the age of quantum computing. Presented at *Acoustical Society of America (ASA) - Fall Meeting*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-26. (LA-UR-22-29154)

Zhang, Y. Non-Adiabatic Modeling of Light-Matter Interactions. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-26. (LA-UR-22-29150)

**Peer-reviewed*

Learn Equations, not Models: Interpretable Digital Twins for Complex Systems

Arvind Mohan
20220567ECR



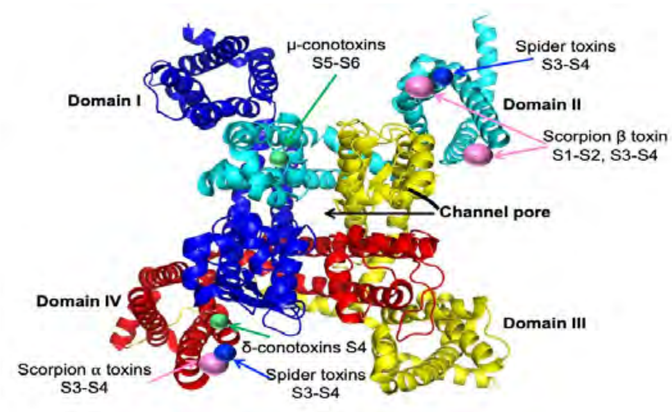
Digital Twins are mathematical clones of complex systems (such as a watershed, in this example). Our digital twin breaks down complex physics equations into an machine learning-driven surrogate model, such that the system response can be quickly forecasted with modest computing resources. Digital twins also utilize real-time measurements from sensors and combine them with the surrogate model to obtain an integrated insight into the system. Such rapid forecasts enable us to use digital twins for disaster response and ecosystem health monitoring, which is otherwise not possible with the full physics equations due to their computational complexity.

Project Description

The United States is facing threats and challenges from multiple sources, especially from natural systems due to the increasingly unreliable climate patterns and energy sources in an uncertain geopolitical environment. A key example of this is the increasing frequency of adverse weather events which need rapid forecasting and active management. Another example is in transportation, such as aviation, where safety is non-negotiable and energy efficiency is essential to reduce reliance on fossil fuels. A promising approach is utilizing mathematical and artificial intelligence (AI) entities called Digital twins, which can perform fast predictions of these systems and assist in quick decision-making to achieve desired outcomes. While AI has been explored for digital twins, it remains unreliable due to the high degree of uncertainty and lack of trust in typical methods that use AI. This project is an ambitious attempt to eliminate this unreliability by supercharging AI with traditional domain knowledge that is accurate, but too slow for rapid decision making. The successful blending of domain knowledge with AI would give us the best of both worlds and tools to help us handle a wide range of problems where continuous monitoring and decision-making are essential for safety and security.

Conotoxins from Omics to Structure to Applications. Large Peptide Libraries and High Throughput Omics to Molecular Structure Analysis Informing Experimental Work in Conotoxins.

Erick LeBrun
20220584ECR



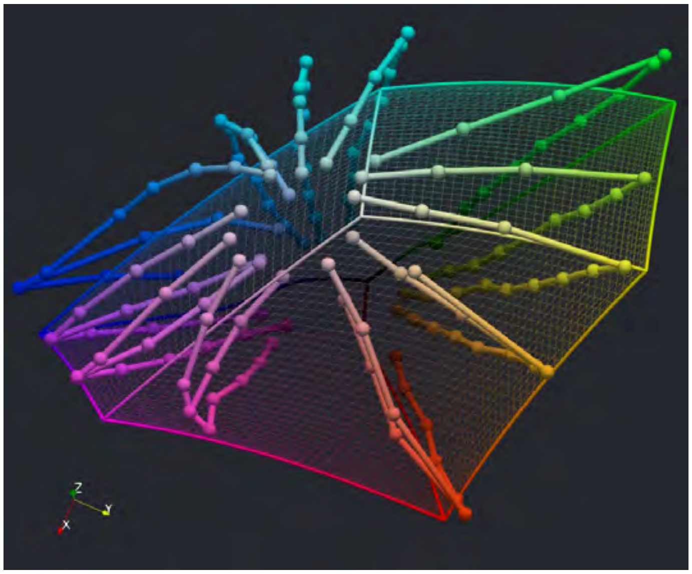
Current classifications of conotoxins are activity-based related to target receptors, disulfide bond composition, and cystine knot scaffolding. LANL is using cutting edge computing methods to better classify and characterize conotoxins based on a combination of their protein sequence as well as their physical structure and atomistic environment.

Project Description

Conotoxins represent a potential reservoir of both beneficial pharmacological molecules and biological threats. Due to their hypervariability and other biological challenges, conotoxins are difficult to study leading to under-classification and under-characterization of the broad grouping of these molecules. Using cutting edge machine learning and molecular dynamic methods along with high throughput in silico screening methods, the broad diversity of conotoxins can be not only better classified, but evaluated for beneficial and deleterious interactions in humas and mammals as well as screened for potential mitigation strategies. These findings can lead to new pharmacological approaches for the use of conotoxins as well as the understanding of potential biological threats associated with conotoxins along with the development of strategies and methods for mitigating identified threats.

Automatic Colormap Improvement in Non-Euclidean Spaces

Roxana Bujack
20200512ECR



In this project, the team will provide algorithms that automatically improve colormaps in non-Euclidean color spaces. The central concept here is the geodesic, i.e. the shortest path between two points. It has long been known that the shortest paths in color space are not straight lines. Now we understand that their length is not even the distance between their endpoints. That means the current paradigm of color space to be Riemannian is not accurate. Color space has an even more complicated shape. The image shows experimentally determined shortest lines of constant hue embedded in the CIELAB color space (defined by the International Commission on Illumination in 1976) limited through the sRGB (standard red, green, blue) gamut.

Project Description

The results of this project can help all application scientists. They depend on scientific visualization for the analysis of their experiments and simulations, for validation and verification and for gaining insight. At Los Alamos, these insights evolve into mission relevant conclusions that are communicated to stakeholders. Colormapping is one of the most common methods to visualize data. A poor colormap hides details or introduces artifacts; a good colormap promotes insight and communication. This project's goal is to extend the interactive Charting Continuous Colormap (CCC) tool (https://ccctool.com) to allow a user to correct and adjust a colormap. This will enable scientists to quickly generate high quality but also customized colormaps. That means that the colormaps will satisfy the specific needs of the scientists, for example, domain conventions, or color constraints due to annotations. At the same time, they will be comparable in quality to carefully designed high quality colormaps.

Technical Outcomes

The project made a revealing discovery that perceptual colorspace cannot be modeled in Riemannian geometry. The project was able to show that the current paradigm which was introduced by Riemann and furthered by Helmholtz and Schroedinger, that perceived color space is a three-dimensional Riemannian space, is incorrect. This results in a paradigm shift that breaks with a 100 year old theory.

Publications

Journal Articles

Bujack, R. B., E. N. Stark, J. M. Miller, E. Caffrey and T. Turton. The non-Riemannian nature of perceptual color space. Submitted to *PNAS*. (LA-UR-21-24630)

Miller, J. M. and R. B. Bujack. Navigating the Gargantua System: Minimal Geodesic Curvature Paths and the Relativistic Transfer. Submitted to *Classical and Quantum Gravity*. (LA-UR-21-24971)

Teti, E. S., T. Turton, J. M. Miller, S. Hong, E. Barenholtz and R. B. Bujack. Validation of Crowdsourced Experiments for Color Perception. Submitted to *Psychological Methods*. (LA-UR-22-22545)

Teti, E. S., T. Turton, J. M. Miller and R. B. Bujack. Maximum Likelihood Estimation of Difference Scaling Functions for Suprathreshold Judgments. Submitted to *Journal of Vision*. (LA-UR-21-31281)

Conference Papers

Bujack, R. B., E. Caffrey, E. N. Stark, T. Turton, D. H. Rogers and J. M. Miller. Efficient Computation of Geodesics in Color Space. Presented at *EuroVis*. (leipzig, Germany, 2023-06-12 - 2023-06-12). (LA-UR-21-24634)

Nardini, P. A., M. Chen, M. Boettinger, G. Scheuermann and R. B. Bujack. Automatic Improvement of Continuous Colormaps in Euclidean Colorspaces. Presented at *EuroVis*. (zurich, Switzerland, 2021-06-14 - 2021-06-14). (LA-UR-19-29080)

Nardini, P. A., M. Chen, R. B. Bujack, M. Boettinger and G. Scheuermann. A Testing Environment for Continuous Colormaps. Presented at *IEEE VIs*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-20-22115)

Reports

Bujack, R. B. Grok Color. Unpublished report. (LA-UR-20-25476)

Bujack, R. B. Visualization Showcases. Unpublished report. (LA-UR-21-29064)

Bujack, R. B., N. W. Birge, V. Geppert-Kleinrath, P. L. Volegov and D. H. Rogers. Topological Analysis for Fusion Ignition. Unpublished report. (LA-UR-21-29431)

Stark, E. N., T. Turton, J. M. Miller and R. B. Bujack. Modeling Color Perception without Assuming Additivity of Color Differences. Unpublished report. (LA-UR-21-24906)

Presentation Slides

Stark, E. N. Diminishing Returns in Color Perception Dissertation Prospectus. . (LA-UR-21-23767)

Teti, E. S. Robotic Olfaction, Human Color Perception, and X-ray Emission Spectroscopy: Victims of "Unfortunate Data". . (LA-UR-21-30342)

Teti, E. S. Diminishing Returns in Color Perception. . (LA-UR-22-21695)

Other

Bujack, R. B. Geodesics in Color Space. Dataset. (LA-UR-21-22239)

Bujack, R. B., E. S. Teti, J. M. Miller, E. Caffrey and T. Turton. Empirical Data from Judgments of Achromatic Color Differences. Dataset. (LA-UR-22-20256)

Teti, E. S., T. Turton, J. M. Miller, E. Barenholtz, S. Hong and R. B. Bujack. Validation of a Crowdsourced Perceptual Study with In-Person Participants. Dataset. (LA-UR-23-22998)

**Peer-reviewed*

Enhancing Bayesian Multivariate Adaptive Regression Spline Models Using Concepts from Deep Learning

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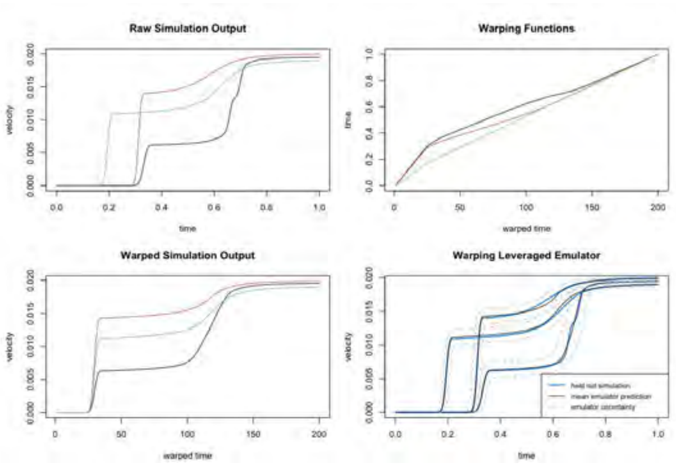


Data with similar general shape, but where important features are misaligned (as shown in the top left plot) are difficult to model with traditional machine learning approaches. When the project team decomposes the misaligned data into aligned data (bottom left plot) and functions that warp the aligned data to the misaligned space (top right plot), accurate modeling can be achieved by modeling the aligned data and warping functions separately and then composing the two resulting machine learning models (predictions shown in bottom right).

Project Description

Machine learning is an important tool in the National Nuclear Security Administration (NNSA) arsenal for addressing many national security challenges, though it has blatant failures. The goal of this project is to combine concepts from the most successful machine learning algorithms with more principled statistical learning models to get accurate, interpretable, and robust new machine learning models that can be trusted in a wider set of circumstances. The potential is for these new models to be useful where other machine learning methods have failed, including some key NNSA mission areas with sparse datasets.

Technical Outcomes

This project developed three new machine learning methods: generalized Bayesian adaptive splines, Bayesian projection pursuit regression, and projected Bayesian adaptive splines. The first two of these are now open source software, while the third is nearing completion. Further, this project also developed a way to interpret Bayesian adaptive splines models using lower dimensional projections. The project was successful in combining concepts from successful machine learning models to get more accurate, interpretable, and robust new models.

Publications

Journal Articles

Collins, G. Q., D. C. Francom and K. N. Rumsey. Bayesian Projection Pursuit Regression. Submitted to *Bayesian Analysis*. (LA-UR-22-21174)

*Francom, D., B. Sanso and A. Kupresanin. Landmark-Warped Emulators for Models with Misaligned Functional Response. 2022. *SIAM/ASA Journal on Uncertainty Quantification*. **10** (1): 125-150. (LA-UR-21-30482 DOI: 10.1137/20M135279X)

Rumsey, K. N., D. C. Francom and A. A. Shen. Generalized Bayesian MARS: Robust, Quantile and Flexible-Likelihood Regression. Submitted to *Journal of the American Statistical Association*. (LA-UR-21-20776)

Rumsey, K. N., S. A. Vander Wiel and D. C. Francom. Discovering Active Subspaces for High Dimensional Computer Models. Submitted to *Journal of Computational and Graphical Statistics*. (LA-UR-22-31726)

Reports

Shen, A. A., K. N. Rumsey and D. C. Francom. TBASS: A Robust Adaptation of Bayesian Adaptive Spline Surfaces. Unpublished report. (LA-UR-20-27873)

Presentation Slides

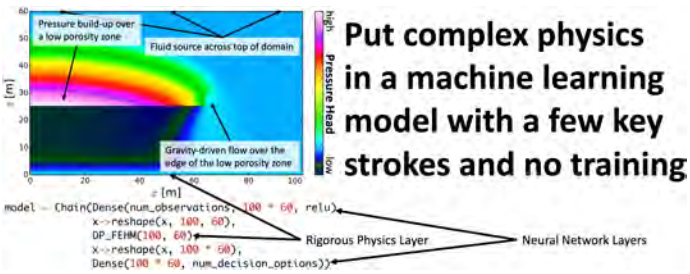
Francom, D. C. Bayesian MARS for efficient and informative nonlinear regression. Presented at *Quality and Productivity Research Conference*, Tallahassee, Florida, United States, 2021-07-26 - 2021-07-26. (LA-UR-21-27269)

Shen, A. A., D. C. Francom and K. N. Rumsey. Robust Bayesian Multivariate Adaptive Regression Splines (BMARS). . (LA-UR-20-27874)

**Peer-reviewed*

Differentiable Programming: Bridging the Gap between Numerical Models and Machine Learning Models

Daniel O'Malley
20200575ECR



This project aims to harness the emerging technology known as Differentiable Programming to develop cutting-edge computational models of complex physics phenomena critical to national security. These models are built in such a way that they can be easily integrated into machine a learning framework, which can reduce the training requirements and make the model more trustworthy.

Project Description

Many national security problems involve components where physical laws are well-understood and other components where the physical laws are either poorly understood or not applicable. Traditional physical models excel at the former whereas interpolating data with machine learning (ML) excels at the latter, but neither approach can tackle these components simultaneously. Existing ML approaches to handling these types of components simultaneously are minor tweaks to standard ML methods. Tweaking black-box ML models is fundamentally limited because "big data does not interpret itself"–meaningful, interpretable structure in models is a necessity to improve predictability, enable human understanding, and maximize the impact of small data. We will meld trustworthy numerical modeling with trainable ML to produce fast models that can thrive on small data through an emerging technology called Differentiable Programming (DP). This project will harness DP to develop cutting-edge computational models of complex physics phenomena critical to national security. Through two applications, we will demonstrate that DP allows us to leverage rigorous physical models in the new paradigm of artificial intelligence (AI)-based science that is being vigorously pursued by Department of Energy (DOE).

Technical Outcomes

The project made significant accomplishments related to each proposal task. This resulted in the release of an open-source subsurface physics simulator that is compatible with machine learning frameworks (pytorch and Flux.jl). The project demonstrated using the simulator to accelerate inverse modeling, and using the simulator combined with machine learning to manage a subsurface fluid injection scenario (carbon dioxide sequestration).

Publications

Journal Articles

*Greer, S. Y., J. D. Hyman and D. O'Malley. A Comparison of Linear Solvers for Resolving Flow in Three-Dimensional Discrete Fracture Networks. 2022. *Water Resources Research*. **58** (4): e2021WR031188. (LA-UR-21-28243 DOI: 10.1029/2021WR031188)

*Harp, D. R., D. O'Malley, B. Yan and R. J. Pawar. On the feasibility of using physics-informed machine learning for underground reservoir pressure management. 2021. *Expert Systems with Applications*. 115006. (LA-UR-21-20260 DOI: 10.1016/j.eswa.2021.115006)

Kadeethum, T., D. O'Malley, F. Ballarin, I. Ang, J. Fuhg, N. Bouklas, V. Silva, P. Salinas, C. Heaney, C. Pain, S. Lee, H. S. Viswanathan and H. Yoon. Accelerating nonlinear solvers with reduced order models. Submitted to *Scientific Reports*. (LA-UR-22-24246)

Kadeethum, T., D. O'Malley, J. N. Fuhg, Y. Choi, J. Lee, H. S. Viswanathan and N. Bouklas. A framework for data-driven solution and parameter estimation of PDEs using conditional generative adversarial networks. Submitted to *Nature Computational Science*. (LA-UR-21-24958)

*Kadeethum, T., F. Ballarin, Y. Choi, D. O'Malley, H. Yoon and N. Bouklas. Non-intrusive reduced order modeling of natural convection in porous media using convolutional autoencoders: Comparison with linear subspace techniques. 2022. *Advances in Water Resources*. **160**: 104098. (LA-UR-21-26841 DOI: 10.1016/j.advwatres.2021.104098)

S. Mehana, M. Z., A. A. Pachalieva, A. Kumar, J. A. Estrada Santos, D. O'Malley, J. W. Carey, M. Sharma and H. S. Viswanathan. Prediction and Uncertainty Quantification of Shale Well Performance Using Multifidelity Monte Carlo. Submitted to *Journal of natural gas Science & Engineering*. (LA-UR-22-28128)

O'Malley, D., S. Y. Greer, A. A. Pachalieva, H. Wu, D. R. Harp and V. V. (. Vesselinov. DPFEHM: a differentiable subsurface physics simulator. Submitted to *Journal of Open Source Software*. (LA-UR-22-28866)

Pachalieva, A., D. O'Malley, D. R. Harp and H. Viswanathan. Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management. 2022. *Scientific Reports*. **12** (1): 18734. (LA-UR-22-24347 DOI: 10.1038/s41598-022-22832-7)

Wu, H., D. O'Malley, J. K. Golden and V. V. Vesselinov. Learning to regularize with a variational autoencoder for hydrogeologic inverse analysis. Submitted to *Advances in Water Resources*. (LA-UR-21-25990)

Wu, H., S. Greer and D. O'Malley. Physics-embedded inverse analysis with algorithmic differentiation for the earth's subsurface. 2023. *Scientific Reports*. **13** (1): 718. (LA-UR-22-27628 DOI: 10.1038/s41598-022-26898-1)

Conference Papers

O'Malley, D., J. A. Estrada Santos and N. E. Lubbers. A Foreign Function Interface for Software 2.0: Automatic Differentiation Across the PyTorch-Julia Barrier. Presented at *AAAI-22 Symposium on Knowledge-Guided ML*. (Arlington, Virginia, United States, 2022-11-17 - 2022-11-19). (LA-UR-22-29477)

Presentation Slides

Kadeethum, T., F. Ballarin, Y. Choi, D. O'Malley, H. Yoon and N. Bouklas. Data-driven solution of natural convection in porous media. Presented at *InterPore*, Online, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25113)

O'Malley, D. Differentiable Programming: Bridging the gap between numerical models and machine learning models. Presented at *Computational Methods in Water Resources*, Online, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30090)

O'Malley, D. Differentiable Programming: Bridging the Gap Between Numerical Models and Machine Learning Models. Presented at *SIAM Geosciences*, Online, New Mexico, United States, 2021-06-21 - 2021-06-21. (LA-UR-21-25809)

O'Malley, D. Differentiable Programming: Bridging the gap between numerical models and machine learning models. Presented at *Machine Learning in Solid Earth Geoscience Lecture*, Online, New Mexico, United States, 2021-10-08 - 2021-10-08. (LA-UR-21-30196)

O'Malley, D. Differentiable Programming: Bridging the gap between numerical models and machine learning models. . (LA-UR-21-31190)

O'Malley, D. PDE constrained optimization and AI. Presented at *Meeting between LANL and AI4Opt*, Online, New Mexico, United States, 2022-02-03 - 2022-02-03. (LA-UR-22-20916)

O'Malley, D. MADS: Motivation and capabilities. Presented at *LANL UQ Tools workshop*, Los Alamos, New Mexico, United States, 2022-06-21 - 2022-06-21. (LA-UR-22-25761)

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O'Malley, D., J. A. Estrada Santos and N. E. Lubbers. Interlingual Automatic Differentiation: Software 2.0 between PyTorch and Julia. Presented at *AAAI Knowledge Guided Machine Learning Symposium*, Arlington, Virginia, United States, 2022-11-17 - 2022-11-17. (LA-UR-22-32115)

Pachalieva, A. A. Physics-informed machine learning for underground reservoir pressure management with heterogeneity. Presented at *American Rock Mechanics Association Annual Meeting*, Santa Fe, New Mexico, United States, 2022-06-26 - 2022-06-26. (LA-UR-22-25825)

Wu, H., D. O'Malley, J. K. Golden and V. V. Vesselinov. Regularization with a variational autoencoder for hydrogeologic inverse analysis. Presented at *Geological Society of America Annual Meeting 2021*, virtual, Oregon, United States, 2021-10-10 - 2021-10-13. (LA-UR-21-29280)

Wu, H. and D. O'Malley. Physics embedded inverse analysis with automatic1 differentiation. . (LA-UR-22-25593)

Posters

Pachalieva, A. A., D. O'Malley, D. R. Harp and H. S. Viswanathan. Physics-Informed Machine Learning with Differentiable Programming for Heterogeneous Underground Reservoir Pressure Management. Presented at *SIAM Conference on Mathematics of Data Science*, San Diego, California, United States, 2022-09-26 - 2022-09-30. (LA-UR-22-28878)

Pachalieva, A. A., D. O'Malley, D. R. Harp and H. S. Viswanathan. Physics-Informed Machine Learning with Differentiable Programming for Heterogeneous Underground Reservoir Pressure Management. Presented at *GRC Flow and Transport in Permeable Media*, Les Diablerets, Switzerland, 2022-07-17 - 2022-07-22. (LA-UR-22-28880)

**Peer-reviewed*

Distributed Algorithms for Large-Scale Ordinary Differential/Partial Differential Equation (ODE/PDE) Constrained Optimization Problems on Graphs

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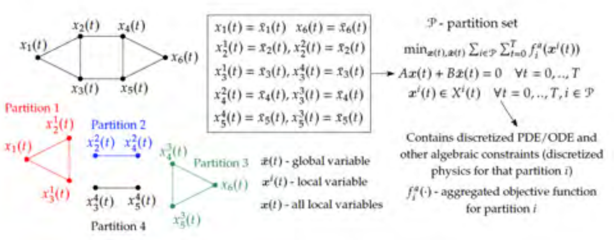
20200603ECR



This project aims to develop a distributed algorithm to solve optimization problems on graphs. The approach leverages graph partitioning techniques to partition the graph (left) and formulate an equivalent problem that can be decomposed and solved in a distributed manner. The convergence of the algorithm and its effectiveness is shown on different applications ranging from energy-infrastructure to surveillance using drones.

Project Description

Analysis of critical infrastructure (natural gas, water, etc.) is a very important national security challenge. The socio-economic systems of the United States depend on the reliable delivery of energy, water, etc. in order to function. As a result, the Department of Energy (DOE) and other stakeholders are tasked with ensuring these systems are safe and robust. However, the ability of policy makers to analyze and protect these systems is limited by the computational requirements of solving related problems in these systems at a nation-wide scale. This project is focused squarely on building the fundamental algorithms that reduce these computational burdens and facilitate the ability of policy makers to make informed decisions on how to best secure the nation's critical infrastructure.

Technical Outcomes

The project made two fundamental contributions to advance algorithms to solve optimization problems that occur in energy infrastucture problems in a nation-wide scale. The first contribution is the development of a distributed algorithm to solve the aforementioned problems that makes effective use of Los Alamos High Performance Computing infrastructure and the second contribution is the development of efficiently solvable surrogate models that can be solved using a standard laptop computer in a matter of seconds.

Publications

Journal Articles

Misra, S., K. Sundar, R. Sharma and K. Brink. Deployable, Data-Driven Unmanned Vehicle Navigation System in GPS-Denied, Feature-Deficient Environments. Submitted to *Journal of Intelligent and Robotic Systems*. (LA-UR-21-20249)

*Rajan, S., K. Sundar and N. Gautam. Routing Problem for Unmanned Aerial Vehicle Patrolling Missions - A Progressive Hedging Algorithm. 2022. *Computers & Operations Research*. **142**: 105702. (LA-UR-21-24769 DOI: 10.1016/j.cor.2022.105702)

Sundar, K., S. Sanjeevi and H. Nagarajan. Sequence of polyhedral relaxations for nonlinear univariate functions. 2022. *Optimization and Engineering*. **23** (2): 877-894. (LA-UR-20-23980 DOI: 10.1007/s11081-021-09609-z)

Sundar, K. and S. Sanjeevi. A Branch-and-Price Algorithm for a Team Orienteering Problem for Fixed-Wing Drones. Submitted to *EURO Journal on Transportation and Logistics*. (LA-UR-19-32483)

Conference Papers

Shin, S., C. J. Coffrin, K. Sundar and V. M. Zavala. Graph-Based Modeling and Decomposition of Energy Infrastructures. Presented at *11th IFAC SYMPOSIUM on Advanced Control of Chemical Processes*. (Venice, Italy, 2021-06-13 - 2021-06-16). (LA-UR-20-27539)

**Peer-reviewed*

Error Correction and Speed-up of Near-term Quantum Computing Architectures

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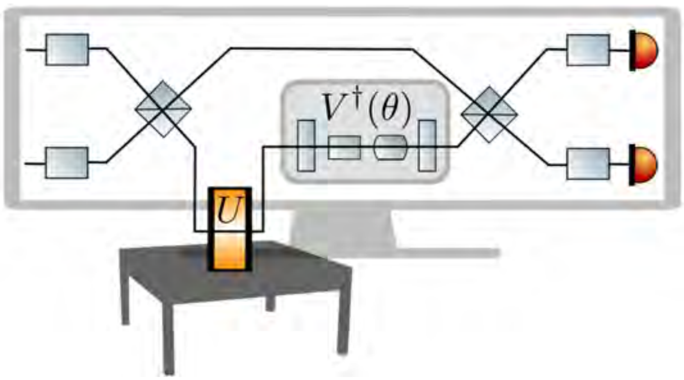
20200677PRD1



Schematic of a variational quantum algorithm (VQA) for compiling a unitary photonic quantum operation U, The VQA generates a high-fidelity approximation of U by coupling to a controllable quantum circuit containing a random parameterized quantum operation V. Photonic squeezing resources (blue rectilinear boxes) are consumed by the VQA and processed by circuit elements that include passive optical operations and photonic measurements. Development and optimization of near-term quantum algorithms such as photonic VQAs is supported by the LDRD program (Image credit: Zoe Holmes, LANL).

Project Description

Quantum computation is an important facet of quantum technology, and constitutes a main focus of the National Quantum Initiative. Highly efficient quantum algorithms implemented in the settings of cryptography, distribution of quantum mechanical resources, and numerical optimization are vital for national information security in an age of quantum technology. The present project analyzes relationships between quantum computer architecture and the potential advantages that the quantum computer can provide, while maintaining an emphasis on near-term quantum devices, such as superconducting, photonic, and atomic quantum processors. This research is immediately applicable to proposed Department of Energy (DOE) missions that require quantum algorithms for enhanced computation and sensing. In particular, the project is focused on designing efficient quantum algorithm modules, which are necessary to exploit the advantages of both intermediate scale and large scale quantum computers.

Publications

*Peer-reviewed

Journal Articles

*Pesah, A., M. Cerezo, S. Wang, T. Volkoff, A. T. Sornborger and P. J. Coles. Absence of Barren Plateaus in Quantum Convolutional Neural Networks. 2021. *Physical Review X*. **11** (4): 041011. (LA-UR-20-29031 DOI: 10.1103/PhysRevX.11.041011)

*Tan, K. C. and T. Volkoff. Variational quantum algorithms to estimate rank, quantum entropies, fidelity, and Fisher information via purity minimization. 2021. *Physical Review Research*. **3** (3): 033251. (LA-UR-21-22998 DOI: 10.1103/PhysRevResearch.3.033251)

Volkoff, T. J. Efficient trainability of linear optical modules in quantum optical neural networks. Submitted to *arXiv*. (LA-UR-20-26436)

Volkoff, T. J. Distillation of maximally correlated bosonic matter from many-body quantum coherence. Submitted to *Quantum*. (LA-UR-20-27370)

Volkoff, T. J. Strategies for variational quantum compiling of a zero-phase beamsplitter on the Xanadu X8 processor. Submitted to *arXiv*. (LA-UR-22-20849)

Volkoff, T. J., J. Ahn, Y. Kwon and J. Kim. Two-dimensional superfluidity in 4He clusters intercalated into graphite. Submitted to *Physical Review B*. (LA-UR-20-29219)

Volkoff, T. J., Z. P. Holmes and A. T. Sornborger. Universal Compiling and (No-)Free-Lunch Theorems for Continuous-Variable Quantum Learning. 2021. *PRX Quantum*. **2** (4): 040327. (LA-UR-21-24060 DOI: 10.1103/PRXQuantum.2.040327)

*Volkoff, T. J. and M. J. Martin. Asymptotic optimality of twist-untwist protocols for Heisenberg scaling in atom-based sensing. 2022. *Physical Review Research*. **4** (1): 013236. (LA-UR-21-23486 DOI: 10.1103/PhysRevResearch.4.013236)

Volkoff, T. J. and M. J. Martin. Saturating the one-axis twisting quantum Cramer-Rao bound with a total spin readout. Submitted to *arXiv*. (LA-UR-22-27372)

Volkoff, T. J. and S. Omanakuttan. Spin squeezed GKP codes for quantum error correction in atomic ensembles. Submitted to *arXiv*. (LA-UR-22-31660)

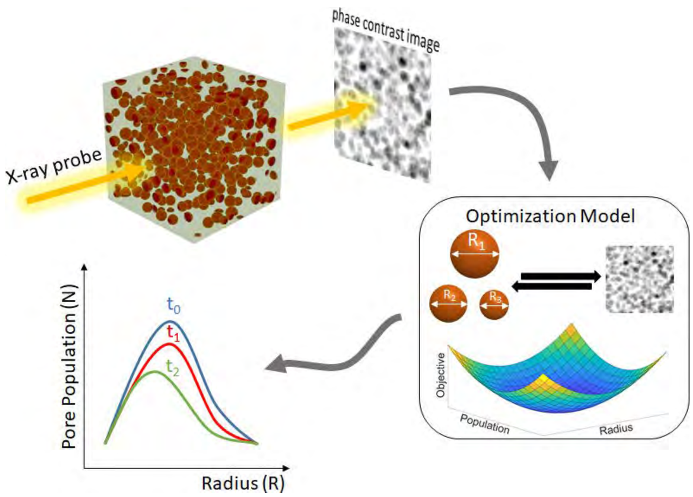
Volkoff, T. J. and S. Omanakuttan. Spin squeezed GKP codes for quantum error correction in atomic ensembles. Submitted to *arXiv*. (LA-UR-22-31877)

Volkoff, T. J. and Y. Suba\xc5\x9f\xc4\xb1. Ancilla-free continuous-variable SWAP test. 2022. *Quantum*. **6**: 800. (LA-UR-22-21141 DOI: 10.22331/q-2022-09-08-800)

*Volkoff, T. and P. J. Coles. Large gradients via correlation in random parameterized quantum circuits. 2021. *Quantum Science and Technology*. **6** (2): 025008. (LA-UR-20-23818 DOI: 10.1088/2058-9565/abd891)

In Situ Quantification of Damage in High Explosives

Pawel Kozlowski
20200744PRD1



Los Alamos researchers are able to gain direct and real-time insight into rapidly evolving granular and porous systems using large scale, high-energy x-ray imaging facilities; however, 2D x-ray images alone are difficult to interpret and quantify. Our project aims to develop optimization models to reconstruct 3D information from a 2D image, and compute evolving particle/pore size distributions. This information will help improve our understanding of the mechanics of interacting particle/pore systems, and it can be applied broadly (e.g., strategy development for safe landing on extraterrestrial soil, porous material behavior and failure, etc.)

Project Description

Understanding materials under extremes, their behavior under dynamic loading, contributions of defects to failure, and how high explosives remain safe under impact are important to Department of Energy/National Nuclear Security Administration missions for advanced material design and modeling materials with computers. Much of our understanding depends on defects in the materials, such as voids and cracks, and how those grow during an extreme event, such as impact. Three-dimensional (3-D) computed tomography, using hundreds of x-ray images from various angles, can measure such defects, but during a dynamic event there is only time for one or a few frames of x-ray images. Using advanced mathematical analysis techniques, prior knowledge of the types of defects, together with the physics of the x-ray image formation process, 3-D information about those defects can be obtained from a single x-ray image. This has been successfully applied to measuring lung alveoli in medical images and to voids in ceramics and will be applied to x-ray images of materials under dynamic loading taken with bright, laser-like x-ray sources in the United States. Such information will help inform and improve our computational models of crack growth and material failure important for security missions, including the nuclear weapons stockpile.

Publications

Journal Articles

Hodge, D. S., A. F. Leong, S. Pandolfi, K. Kurzer-Ogul, D. S. Montgomery, H. Aluie, C. Bolme, T. Carver, E. Cunningham, C. B. Curry, M. Dayton, F. Decker, E. Galtier, P. Hart, D. Khaghani, H. J. Lee, K. Li, Y. Liu, K. Ramos, J. Shang, S. Vetter, B. Nagler, R. L. Sandberg and A. E. Gleason. Multi-frame, ultrafast, x-ray microscope for imaging shockwave dynamics. 2022. *Optics Express*. **30** (21): 38405-38422. (LA-UR-22-26397 DOI: 10.1364/OE.472275)

Leong, A. F., C. M. Romick, D. Montgomery, K. J. Ramos, C. A. Bolme and T. D. Aslam. Quantitative X-ray Phase contrast Imaging of Oblique Shock Waves. Submitted to *Journal of Applied Physics*. (LA-UR-22-25472)

Pandolfi, S., T. Carver, D. Hodge, A. F. T. Leong, K. Kurzer-Ogul, P. Hart, E. Galtier, D. Khaghani, E. Cunningham, B. Nagler, H. J. Lee, C. Bolme, K. Ramos, K. Li, Y. Liu, A. Sakdinawat, S. Marchesini, P. M. Kozlowski, C. B. Curry, F. Decker, S. Vetter, J. Shang, H. Aluie, M. Dayton, D. S. Montgomery, R. L. Sandberg and A. E. Gleason. Novel fabrication tools for dynamic compression targets with engineered voids using photolithography methods. 2022. *Review of Scientific Instruments*. **93** (10): 103502. (LA-UR-22-31504 DOI: 10.1063/5.0107542)

Presentation Slides

Leong, A. F. Characterizing the Dynamic Behavior of Porous Materials using X-ray Phase Contrast Imaging. Presented at *Physics Cafe (Virtual)*, Los Alamos, New Mexico, United States, 2021-07-22 - 2021-07-22. (LA-UR-21-27962)

Leong, A. F. Distribution measurement of micron-size features from XPCI images in the near-field to Fresnel regime. Presented at *Enabling 3D mesoscale imaging under dynamic conditions (Virtual)*, Los Alamos, New Mexico, United States, 2021-09-14 - 2021-09-16. (LA-UR-21-29033)

Leong, A. F., B. Zuanetti, M. Zecevic, K. J. Ramos, C. A. Bolme, C. Meredith, J. L. Barber, M. J. Cawkwell, B. E. Wohlberg, M. T. McCann, T. C. Hufnagel, P. M. Kozlowski and D. Montgomery. PBX9502: Connecting 3D Microstructure to Sub-shock Detonation using X-ray Phase Contrast Imaging. Presented at *MACH Conference*, Baltimore, Maryland, United States, 2023-04-05 - 2023-04-07. (LA-UR-23-23394)

Leong, A. F., B. Zuanetti, M. Zecevic, K. J. Ramos, C. A. Bolme, C. S. Meredith, J. L. Barber, M. J. Cawkwell, B. E. Wohlberg, M. T. McCann, T. C. Hufnagel, P. M. Kozlowski and D. Montgomery. In-situ Mesoscale Characterization of Dynamic Crack Initiation and Propagation using X-ray Phase Contrast Imaging. Presented at *SEM Annual Conference and Exposition*, Orlando, Florida, United States, 2023-06-05 - 2023-06-08. (LA-UR-23-21700)

Leong, A. F., C. M. Romick, T. D. Aslam, C. A. Bolme, D. Montgomery and K. J. Ramos. Quantitative methods for studying shock-material behavior using x-ray phase contrast imaging. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26408)

Leong, A. F., C. M. Romick, T. D. Aslam, C. A. Bolme, D. Montgomery and K. J. Ramos. Quantitative methods for studying shock-material behavior using x-ray phase contrast imaging. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26596)

Leong, A. F., E. Asare, V. Kannan, Q. Zeng, D. Montgomery, K. Ramesh and T. Hufnagel. Evolution of pore size distribution of sandstone under dynamic loading. . (LA-UR-23-21280)

Pandolfi, S., A. Gleason, H. Lee, B. Nagler, E. Galtier, E. Cunningham, Y. Liu, S. Marchesini, K. Li, A. Sakdinawat, P. Hart, C. Curry, M. H. Seaberg, D. Khaghani, S. L. Vetter, F. J. Decker, W. Mao, T. Carver, R. Sandberg, D. S. Hodge, M. Ricks, C. McCombs, N. Blanchard, D. Montgomery, C. A. Bolme, P. M. Kozlowski, K. J. Ramos, M. S. Powell, A. F. Leong, S. Ali, P. Celliers, M. Dayton, L. Dresselhaus-Marais, T. Doeppner, L. D. Claus and M. O. Sanchez. Ultrafast time-resolved imaging of void collapse in ICF ablator materials. Presented at *APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-31420)

Posters

Leong, A. F., D. S. Hodge, S. Pandolfi, Y. Liu, K. Li, A. Sakdinawat, E. Galtier, B. Nagler, H. J. Lee, E. Cunningham, C. A. Bolme, K. J. Ramos, P. M. Kozlowski, D. Khaghani, T. Carver, S. Marchesini, R. Sandberg, A. Gleason and D. Montgomery. Speckle-based X-ray Phase Contrast Imaging at Free-Electron Lasers. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, Maryland, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26435)

Leong, A. F., D. S. Hodge, S. Pandolfi, Y. Liu, K. Li, A. Sakdinawat, E. Galtier, B. Nagler, H. J. Lee, E. Cunningham, C. A. Bolme, K. J. Ramos, P. M. Kozlowski, D. Khaghani, T. Carver, S. Marchesini, R. L. Sandberg, A. Gleason and D. Montgomery. Speckle-based X-ray Phase Contrast Imaging at Free-Electron Lasers. Presented at *2022 SSRL/LCLS USERS*, Online, New Mexico, United States, 2022-09-26 - 2022-09-30. (LA-UR-22-29633)

Leong, A. F., D. S. Hodge, S. Pandolfi, Y. Liu, K. Li, A. Sakdinawat, E. Galtier, B. Nagler, H. J. Lee, E. Cunningham, C. A. Bolme, K. J. Ramos, P. M. Kozlowski, D. Khaghani, T. Carver, S. Marchesini, R. L. Sandberg, A. Gleason and D. Montgomery. Speckle-based X-ray Phase Contrast Imaging at Free-Electron Lasers. Presented at *Ulitima conference*, Menlo Park, California, United States, 2023-03-13 - 2023-03-16. (LA-UR-23-22546)

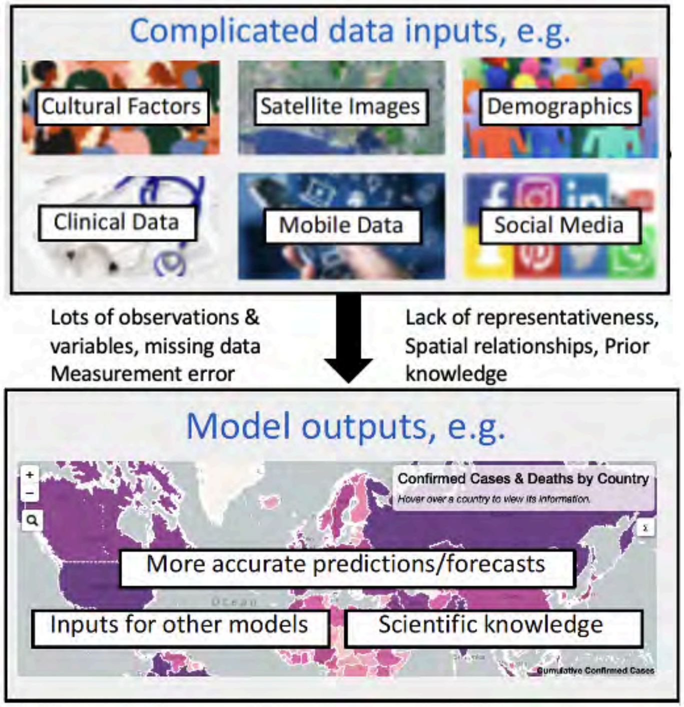
Leong, A. F., K. Hom, R. Agyei, A. Zare, T. Hufnagel and L. Li. Characterization of Geomaterials before and during dynamic loading. Presented at *Materials science in extreme environments university research alliance annual technical review*, Baltimore, Maryland, United States, 2022-06-22 - 2022-06-24. (LA-UR-22-25624)

Montgomery, D., A. F. Leong, J. L. Barber, C. A. Bolme and K. J. Ramos. In situ phase contrast imaging for cracks and voids under dynamic loading. Presented at *2021 Conventional High Explosives Grand Challenge (CHEGC) Technical Symposium*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-10. (LA-UR-21-31792)

**Peer-reviewed*

Addressing Data Challenges to Improve Prediction Models

Lauren VanDervort
20210761PRD1



Schematic diagram describing the data challenges addressed through the work of this project. The project goal is to apply and extend statistical approaches to address data challenges and develop strategies for combining useful but messy, complicated inputs to generate knowledge that can be applied to model forecasting.

Project Description

Methodologies for fusing disparate data streams that can address sparse, misclassified, and missing data are critical for addressing many mission-relevant problems to address emerging and reemerging threats for the Nation. This project will do exactly that by developing approaches that can digest real-time data while correcting for their limitations to increase the reliability of models and forecasts.

Publications

Journal Articles

*Beesley, L. J., D. Osthus and S. Y. Del Valle. Addressing delayed case reporting in infectious disease forecast modeling. 2022. *PLOS Computational Biology*. **18** (6): e1010115. (LA-UR-21-30640 DOI: 10.1371/journal.pcbi.1010115)

VanDervort, L. J. COVID-19 Outcomes by Cancer Status, Site, Treatment, and Vaccination. 2023. *Cancer Epidemiology, Biomarkers & Prevention*. (LA-UR-22-21557 DOI: 10.1158/1055-9965.EPI-22-0607)

VanDervort, L. J. Case studies in bias reduction and inference for electronic health record data with selection bias and phenotype misclassification. 2022. *Statistics in Medicine*. (LA-UR-22-23875 DOI: 10.1002/sim.9579)

VanDervort, L. J., D. A. Osthus, E. M. Casleton, P. L. Lafreniere, R. C. Johns, K. Dayman, J. Hite, O. Marcillo, M. Maceira, E. Cardenas, D. Chinchester, D. Archer, J. Ghawaly, I. Garishvili, A. Rowe, I. Stewart and M. Willis. Integrating seismic, infrasound, and radiation data to characterize movements of nuclear materials. Submitted to *INMM Conference Proceedings*. (LA-UR-22-26225)

VanDervort, L. J., D. A. Osthus, K. R. Moran, M. A. Ausdemore, G. D. Meadors, P. H. Janzen, B. P. Weaver and D. B. Reisenfeld. Statistical methods for partitioning ribbon and globally distributed flux using data from the Interstellar Boundary Explorer. Submitted to *Journal of the American Statistical Association*. (LA-UR-22-32267)

VanDervort, L. J., K. R. Moran, K. Wagh, L. A. Castro, J. P. Theiler, H. Yoon, W. M. Fischer, N. W. Hengartner, B. T. M. Korber and S. Y. Del Valle. SARS-CoV-2 variant transition dynamics are associated with vaccination rates, number of co-circulating variants, and natural immunity. Submitted to *Lancet Infectious Diseases*. (LA-UR-22-32123)

VanDervort, L. J., M. Abbott, E. Bellile, A. Shuman, L. Rozek and J. M. G. Taylor. Comparing individualized survival predictions from random survival forests and multistate models: a case study of patients with oropharyngeal cancer. Submitted to *Statistics in Medicine*. (LA-UR-22-24202)

VanDervort, L. J., P. Patelli, J. P. Schwenk, K. M. Martinez, T. R. Pitts, M. J. Barnard, K. A. Kaufeld, B. H. Mcmahon and S. Y. Del Valle. Multi-dimensional resilience: A quantitative exploration of disease outcomes and economic, political, and social resilience to the COVID-19 pandemic in six countries. 2023. *PLOS ONE*. **18** (1): e0279894. (LA-UR-21-31106 DOI: 10.1371/journal.pone.0279894)

Reports

VanDervort, L. J. Imputation of SARI Time Series. Unpublished report. (LA-UR-22-20223)

Presentation Slides

Osthus, D. A., L. J. VanDervort and S. Y. Del Valle. Addressing delayed case reporting for infectious disease models. . (LA-UR-21-27812)

VanDervort, L. J. Web Tool for Outcome Prognostication in Patients Newly-Diagnosed with Oropharyngeal Cancer. . (LA-UR-21-30661)

VanDervort, L. J. Measurement Error, Selection Bias, and Missing Data in Biomedical Research. Presented at *CCS-6 Seminar*, Los Alamos, New Mexico, United States, 2021-11-17 - 2021-11-17. (LA-UR-21-31246)

VanDervort, L. J. Statistics at Los Alamos National Laboratory. Presented at *Virtual Student seminar at University of Michigan Department of Biostatistics*, Ann Arbor, Michigan, United States, 2022-01-28 - 2022-01-28. (LA-UR-22-20528)

VanDervort, L. J. Primer on Ribbon Separation. . (LA-UR-22-20511)

VanDervort, L. J. Statistical inference for association studies using EHR: handling both selection bias and outcome misclassification. Presented at *University of Colorado Invited Seminar (Virtual)*, Los Alamos, New Mexico, United States, 2022-02-14 - 2022-02-14. (LA-UR-22-20963)

VanDervort, L. J. Ribbon Center Estimation and Ribbon Separation. . (LA-UR-22-23409)

VanDervort, L. J. Ribbon center estimation and ribbon separation. Presented at *IBEX LDRD Data Analysis Meeting*, Los Alamos, New Mexico, United States, 2022-06-21 - 2022-06-21. (LA-UR-22-25845)

VanDervort, L. J. Integrating seismic, infrasound, and radiation data to characterize movements of nuclear materials. Presented at *Institute of Nuclear Materials Management*, Los Alamos, New Mexico, United States, 2022-07-25 - 2022-07-25. (LA-UR-22-27412)

VanDervort, L. J. A Global Comparison of COVID-19 Variant Waves and Relationships with Clinical and Demographic Factors. Presented at *NIH COVID Tracking Team Meeting*, Los Alamos, New Mexico, United States, 2022-09-12 - 2022-09-12. (LA-UR-22-29278)

VanDervort, L. J. IBEX Update. . (LA-UR-22-29818)

VanDervort, L. J. Ribbon separation and center estimation for IBEX data. Presented at *IMAP Mission Meeting*, Santa Fe, New Mexico, United States, 2022-10-27 - 2022-10-28. (LA-UR-22-31074)

VanDervort, L. J. Statistics at Los Alamos National Laboratory. . (LA-UR-23-20196)

VanDervort, L. J., D. A. Osthus and S. Y. Del Valle. Addressing Data Challenges to Improve Prediction Models: Progress Update, Sept. 2021. . (LA-UR-21-29302)

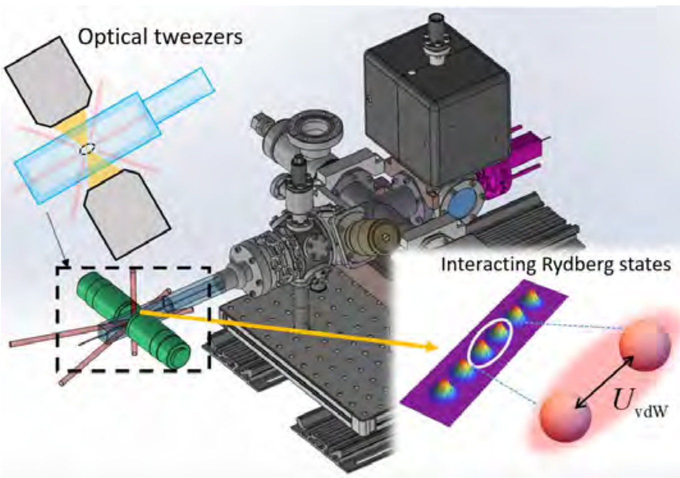
Posters

VanDervort, L. J., D. A. Osthus, K. R. Moran, M. A. Stricklin, G. D. Meadors, P. H. Janzen, E. Zirnstein, B. P. Weaver and D. B. Reisenfeld. Statistical methods for partitioning ribbon and globally-distributed flux using data from the Interstellar Boundary Explorer. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-10. (LA-UR-23-21987)

**Peer-reviewed*

Quantum Information with Atoms in Optical Tweezers

Michael Martin
20210955PRD3



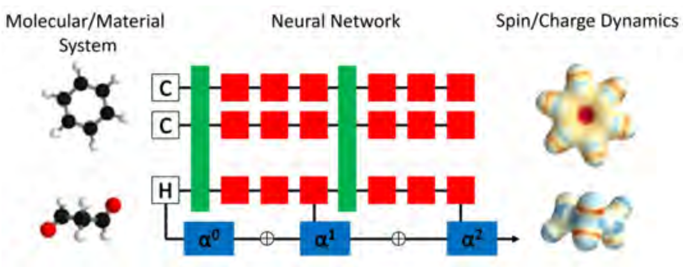
Optical Tweezers (top left inset) allow manipulation of single atoms for entanglement (bottom right inset). The technique benefits a wide range of experiments with ultracold neutral atoms.

Project Description

The subcommittee on Quantum Information Science under the Committee on Science of the National Science and Technology Council published a report in September 2018 entitled “National Strategic Overview for Quantum Information Science.” Here, the economic and defense implications of quantum systems are discussed. Cited applications included optimization problems, chemistry, sensing, and machine learning. An outstanding challenge is to discover new systems and approaches that might one day impact these applications. Neutral atom systems, as developed here, are one promising approach, and sensing advantages may be imminent. This work will explore a system comprising interacting qubits encoded in individual neutral atoms, with a specific emphasis on an enabling technology: optical tweezers. First, we will develop a trapping strategy to elucidate the coherence and entanglement advantages of qubits stored in the nucleus of the alkaline earth atom strontium-87. Second, and in parallel, we will develop a robust method for entangling a single atom with a Bose-Einstein condensate sensor, which has the potential to increase sensor performance as well as explore fundamental questions relating to quantum correlations and entanglement.

AI-Enabled Electron Dynamics at the Device Scale

Benjamin Nebgen
20210956PRD3



Architecture of Los Alamos National Laboratory developed Hierarchically Interacting Particle Neural Network (HIPNN) making predictions of wavefunction information on molecular systems. The goal of this project is to extend this neural network to make dynamic predictions on spin and electron transport during a molecular dynamics simulation.

Project Description

The reduced computational cost of machine learning (ML) models for modeling electron dynamics would facilitate the simulation of million atom systems, allowing for first principles modeling of electron interactions with phonons, defects, surfaces and interfaces across entire devices. The computational framework will be inclusive of device complexities, for example, having solid-solid or solid-molecule interfaces and various types of defects. This will be useful for various projects central to Los Alamos National Laboratory's interest, e.g. energy conversion, bio-sensing, drug design and computation. Importantly, with the developed methodology will be critical for the formation of effective collaborations with researchers at Los Alamos (e.g. Center for Integrated nanotechnologies) whose work closely focus on two rapidly developing fields at the forefront of novel technologies: efficient plasmon driven hot carrier energy harvesting devices, and modeling the manipulation of electron spin states in promising materials for quantum computation and communication. For the broader scientific community, this device-scale electron dynamics will provide researchers the much-needed platform to understand the fundamental physical limitations present in the design of efficient technologies.

Publications

Journal Articles

Habib, A., J. Xu, Y. Ping and R. Sundararaman. Electric fields and substrates dramatically accelerate spin relaxation in graphene. Submitted to *Physical Review B*. (LA-UR-22-24378)

Habib, A., N. E. Lubbers, S. Tretiak and B. T. Nebgen. Machine learning models capture plasmon dynamics in Ag nanoparticles. Submitted to *Journal of Physical Chemistry C*. (LA-UR-22-32313)

Habib, A., R. Sundararaman, J. Xu, H. Takenaka and Y. Ping. Giant Spin Lifetime Anisotropy and Spin-Valley Locking in Silicene and Germanene from First-Principles Density-Matrix Dynamics. Submitted to *Nano Letters*. (LA-UR-21-30731)

Presentation Slides

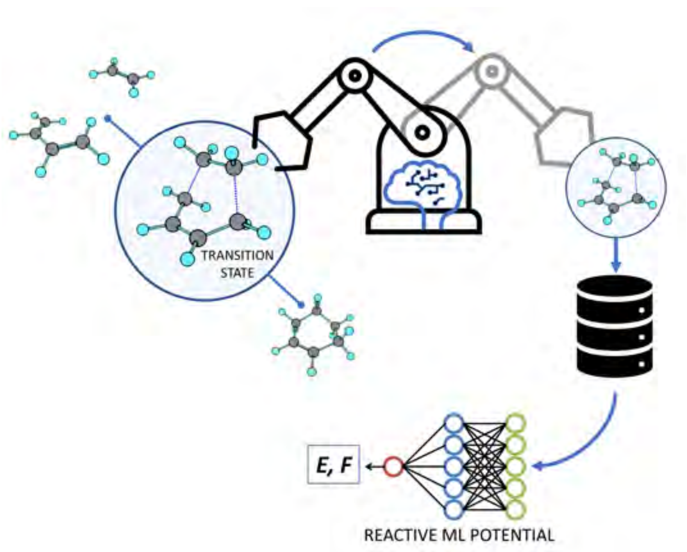
Habib, A. Atomistic Simulation of Plasmonic Hot Carrier Dynamics Using Machine Learning. Presented at *CNLS - Physic Informed Machine Learning*, Santa Fe, New Mexico, United States, 2022-05-11 - 2022-05-13. (LA-UR-22-24377)

Habib, A., B. T. Nebgen, N. E. Lubbers and S. Tretiak. Predictions of Plasmonic Hot Carrier Energies Using Machine Learning. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22295)

**Peer-reviewed*

Atomic-Scale Machine Learning for Catalysis and Reactive Chemistry

Benjamin Nebgen
20220793PRD2



Recent advances have proven that machine learning (ML) atomistic potentials strike a balance between QM accuracy and force field speed. However, such potentials lack chemical reactivity which is crucial in many LANL-relevant large-scale applications, such as detonation chemistry, phase transitions, shock physics, and materials aging. Chemical-space sampling methods involving reinforcement learning, assisted by dimensionality reduction techniques, will help to prioritize statistically-rare atomistic structures (such as transition states or activated complexes) where data is sparse. This approach will help to collect datasets comprising rare reactive states and train highly-accurate reactive ML potentials applicable in catalytic processes.

Project Description

Despite the growing use of Machine Learning in chemistry and materials science, its application to catalysis is still in the early stages. By leveraging Los Alamos National Lab's computational resources, group members' experience, and Los Alamos developed codes, this project will produce a framework for generating high-quality data of statistically-rare atomistic structures, underpinning catalytic reactions. The methods developed in this project also have a variety of applications to mission relevant materials such as explosives and shocked materials. Additionally, the developed framework will be utilized to search for novel cayalysis for Fischer-Tropsch synthesis, a method by which carbon monoxide (a waste product from combustion engines), water and hydrogen are reacted to produce industrial useful hydrocarbons.

Publications

Journal Articles

Fedik, N., B. T. Nebgen, N. E. Lubbers, K. M. Barros, M. Kulichenko, Y. W. Li, R. Zubatyuk, R. A. Messerly, O. Isayev and S. Tretiak. Synergy of Semiempirical Models and Machine Learning in Computational Chemistry. Submitted to *Journal of Chemical Physics*. (LA-UR-23-23011)

Kulichenko, M., K. M. Barros, N. E. Lubbers, N. Fedik, G. Zhou, S. Tretiak, B. T. Nebgen and A. M. Niklasson. Semi-Empirical Shadow Molecular Dynamics: A PyTorch implementation. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-22-33200)

Kulichenko, M., K. M. Barros, N. E. Lubbers, Y. W. Li, R. A. Messerly, S. Tretiak, J. S. Smith and B. T. Nebgen. Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials. Submitted to *Nature Computational Science*. (LA-UR-22-30360)

Kulichenko, M., N. E. Lubbers, J. Smith, Y. W. Li, R. A. Messerly, S. Tretiak, K. M. Barros and B. T. Nebgen. Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials.. Submitted to *Nature Computational Science*. (LA-UR-22-29407)

Pozdeev, A. S., W. Chen, M. Kulichenko, H. W. Choi, A. I. Boldyrev and L. S. Wang. On the Structures and Bonding of Copper Boride Nanoclusters, Cu2Bx- (x = 5-7). Submitted to *Solid State Sciences*. (LA-UR-23-22187)

Presentation Slides

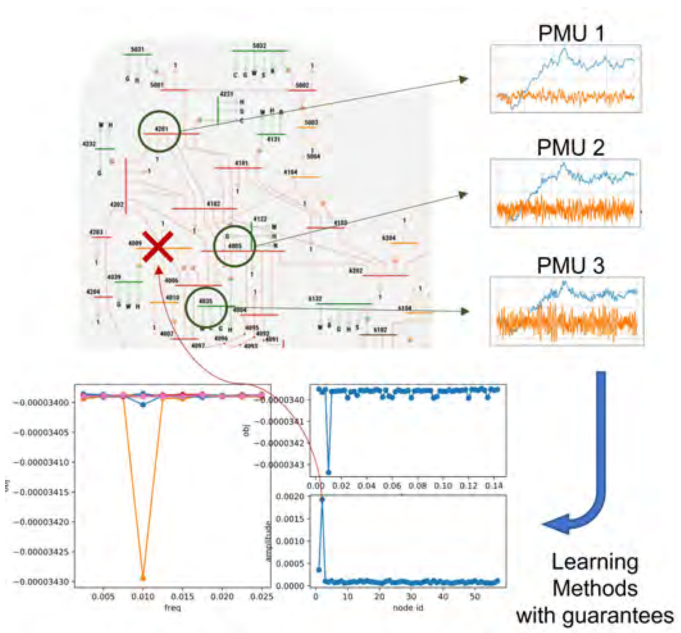
Kulichenko, M. Accelerating Data Generation for Machine Learning Potentials by Biasing Towards Regions of Uncertainty. Presented at *International Conference on Chemical Bonding*, Kapaa, Hawaii, United States, 2022-08-11 - 2022-08-11. (LA-UR-22-28212)

Kulichenko, M. Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials.. Presented at *Machine Learning and Informatics for Chemistry and Materials*, Telluride, Colorado, United States, 2022-10-03 - 2022-10-03. (LA-UR-22-30315)

**Peer-reviewed*

Fault Identification and Inference in Complex Networked Systems

Marc Vuffray
20220797PRD2



By observing at various locations the dynamic of complex networks (here a power grid), a perturbation (shown in red) caused by a malfunctioning component is detected and localized before it can damage the integrity of the network thanks to our newly developed algorithm. Through the work of this project the team will create mathematical tools that can quickly identify sources of perturbations in the dynamic of networks.

Project Description

One of the core missions of the Department of Energy is to ensure safe and reliable energy delivery across the United States. The outcomes of this project will lead to new ways to find undesirable sources of perturbations that are detrimental to the lifespan of vital assets in critical infrastructure networks such as power transmission and distribution grids and natural gas networks. This challenge is especially important to tackle today for the increasing penetration of renewable energy in our energy delivery networks introduces more source of uncertainty and perturbations.

Publications

Journal Articles

Delabays, R., A. Lokhov, M. S. Tyloo and M. D. Vuffray. Locating the source of forced oscillations in transmission power grids. Submitted to *Nature Energy*. (LA-UR-22-32412)

*Delabays, R., L. Pagnier and M. Tyloo. Locating fast-varying line disturbances with the frequency mismatch. *IFAC-PapersOnLine*. **55** (13): 270-275. (LA-UR-22-25502 DOI: 10.1016/j.ifacol.2022.07.271)

Delabays, R. and M. S. Tyloo. Heavy-tailed distribution of the number of papers within scientific journals. 2022. *Quantitative Science Studies*. 1-17. (LA-UR-22-30310 DOI: 10.1162/qss_a_00201)

*Jacquod, P. and M. Tyloo. Propagation of non-Gaussian voltage angle fluctuations in high-voltage power grids. *IFAC-PapersOnLine*. **55** (13): 67-72. (LA-UR-22-25503 DOI: 10.1016/j.ifacol.2022.07.237)

*Tyloo, M. Layered complex networks as fluctuation amplifiers. 2022. *Journal of Physics: Complexity*. **3** (3): 3. (LA-UR-22-23661 DOI: 10.1088/2632-072X/ac7e9d)

Tyloo, M. S. Faster network disruption from layered oscillatory dynamics. 2022. *Chaos: An Interdisciplinary Journal of Nonlinear Science*. **32** (12): 121102. (LA-UR-22-30194 DOI: 10.1063/5.0129123)

Tyloo, M. S., J. Hindes and P. Jacquod. Finite-time correlations boost large voltage angle fluctuations in electric power grids. 2023. *Journal of Physics: Complexity*. (LA-UR-22-25645 DOI: 10.1088/2632-072X/acb62a)

Conference Papers

Tyloo, M. S. Assessing the impact of Byzantine attacks on coupled phase oscillators. Presented at *IEEE Conference on Decision and Control*. (Singapore, Singapore, 2023-12-13 - 2023-12-15). (LA-UR-23-23095)

Presentation Slides

Tyloo, M. S. More complexity for richer network dynamics. Presented at *CNLS Postdoc Seminar*, Los Alamos, New Mexico, United States, 2022-08-18 - 2022-08-18. (LA-UR-22-28806)

Tyloo, M. S. Noise Transmission in Layered Complex Networks. Presented at *COMPLEX NETWORKS 2022 The 11th International Conference on Complex Networks and their Applications*, Palermo, Italy, 2022-11-08 - 2022-11-10. (LA-UR-22-30069)

Tyloo, M. S. Heavy-tailed distribution of the number of papers within scientific journals. Presented at *CNLS Postdoc seminar*, Los Alamos, New Mexico, United States, 2022-10-20 - 2022-10-20. (LA-UR-22-30931)

Tyloo, M. S. Noise Transmission and Disruption in Layered Complex Networks. Presented at *Visit University of Naples Federico II, Italy*, Naples, Italy, 2022-11-11 - 2022-11-16. (LA-UR-22-31747)

Tyloo, M. S. Locating the source of forced oscillations in complex oscillator networks and power grids. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-21609)

Posters

Delabays, R., A. Lokhov, M. S. Tyloo and M. D. Vuffray. Locating the source of forced oscillations in transmission grids. Presented at *gridscience*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-13. (LA-UR-22-32849)

Delabays, R., L. Pagnier and M. S. Tyloo. Locating fast-varying line disturbances with the frequency mismatch. Presented at *IFAC Conference on Networked Systems, NecSys22*, Zurich, Switzerland, 2022-07-05 - 2022-07-07. (LA-UR-22-25459)

Jacquod, P. and M. S. Tyloo. Propagation of non-Gaussian voltage angle fluctuations in high-voltage power grids. Presented at *IFAC Conference on Networked Systems, NecSys22*, Zurich, Switzerland, 2022-07-05 - 2022-07-07. (LA-UR-22-26072)

Tyloo, M. S. Primary control effort and noise propagation in high-voltage power grids. Presented at *The 5th Autonomous Energy System Workshop at NREL*, Golden, Colorado, United States, 2022-07-13 - 2022-07-15. (LA-UR-22-25665)

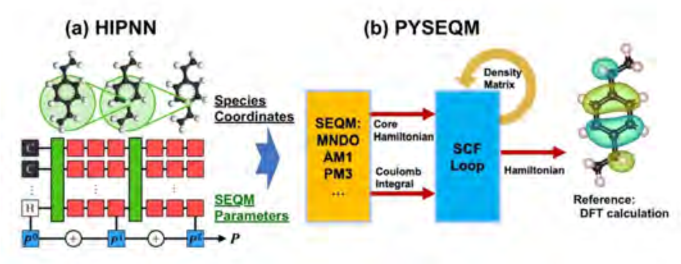
Tyloo, M. S. Fluctuations in Layered Complex Networks. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-02-10. (LA-UR-23-21608)

**Peer-reviewed*

Excited State Dynamics: Improving Hamiltonians with Machine Learning

Sergei Tretiak

20220801PRD3



Model structure scheme. (a) Neural network, HIPNN, with molecular configurations as input (black and white blocks), interacting layers (green blocks), onsite layers (red blocks) and inference layers (blue blocks). (b) The quantum mechanical PYSEQM module takes molecule configurations from HIPNN to generate Hamiltonian. Backpropagation through the entire procedures enables stochastic gradient descent training to reference data

Project Description

The project aims to develop physical models that retain quantum mechanical description of materials using machine learning algorithms. These models will enable accurate simulations of functional materials including molecular switches and miniature data storage, photocatalytic and photovoltaic systems, energy-conserving materials, optical quantum materials, and light-sensitive explosives.

Publications

Journal Articles

Fedik, N., B. T. Nebgen, N. E. Lubbers, K. M. Barros, M. Kulichenko, Y. W. Li, R. Zubatyuk, R. A. Messerly, O. Isayev and S. Tretiak. Synergy of Semiempirical Models and Machine Learning in Computational Chemistry. Submitted to *Journal of Chemical Physics*. (LA-UR-23-23011)

Fedik, N., R. Zubatyuk, M. Kulichenko, N. E. Lubbers, S. J. Smith, B. T. Nebgen, R. A. Messerly, Y. W. Li, A. I. Boldyrev, K. M. Barros, O. Isayev and S. Tretiak. Extending machine learning beyond intleratomic potentials for predicting molecular properties. Submitted to *Nature Reviews Chemistry*. (LA-UR-22-31287)

Gibson, T. R., V. M. Freixas, W. F. I. Malone, X. Li, H. Song, H. Negrin-Yuvero, A. J. White, D. V. Makhov, D. Shalashilin, Y. Zhang, N. Fedik, M. Kulichenko, R. A. Messerly, L. Mohanam, S. Fernandez-Alberti and S. Tretiak. NEXMD2 Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-23-20313)

Kulichenko, M., K. M. Barros, N. E. Lubbers, N. Fedik, G. Zhou, S. Tretiak, B. T. Nebgen and A. M. Niklasson. Semi-Empirical Shadow Molecular Dynamics: A PyTorch implementation. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-22-33200)

Presentation Slides

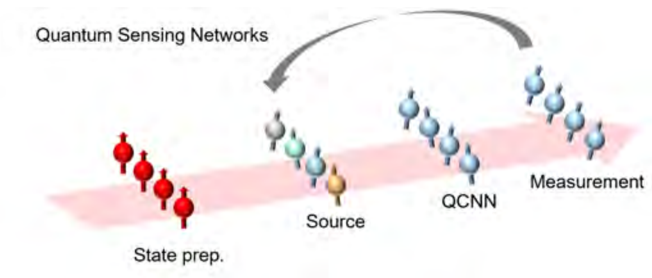
Fedik, N. S. Machine Learning Beyond Interatomic Potentials for Predicting Molecular Properties. Presented at *International Conference on Chemical Bonding 2022*, Kauai, Hawaii, United States, 2022-08-11 - 2022-08-16. (LA-UR-22-28390)

Fedik, N. S. Machine Learning Chemical Properties Along the Atomistic Scale. Presented at *Machine Learning and Informatics for Chemistry and Materials*, Telluride, Colorado, United States, 2022-10-03 - 2022-10-07. (LA-UR-22-30138)

**Peer-reviewed*

Quantum Machine Learning for Quantum Sensing Networks

Andrew Sornborger
20220803PRD3



The quantum sensing network scheme starts with the preparation of a well-known state which interacts with a source that imprints a number of characteristics on the system. Leveraging tools from quantum machine learning, particularly Quantum Convolutional Neural Networks (QCNN), one can measure and learn properties of the system at hand. Via repetition of the learning process, one obtains successively better characterizations of the quantum system being sensed, which leads to more optimal measurements of the system.

Project Description

Quantum sensing, used to measure system properties with high precision, has applications in a wide range of fields such as measurements of electric or magnetic fields, temperature, dark matter detection and gravitational waves. As such, quantum sensing has broad relevance to many areas of interest for the Nation. In order to improve our quantum sensing capabilities, we leverage tools from quantum machine learning to develop protocols for more complex scenarios, that is, extending quantum sensing protocols from measuring a single property of a system to measuring multiple parameters of a quantum system simultaneously.

Publications

Presentation Slides

Huerta Alderete, C. Inference-based quantum sensing: a data-driven approach. Presented at *IQuS Workshop: At the Interface of Quantum Sensors and Quantum Simulations*, Seattle, Washington, United States, 2022-11-07 - 2022-11-18. (LA-UR-22-31768)

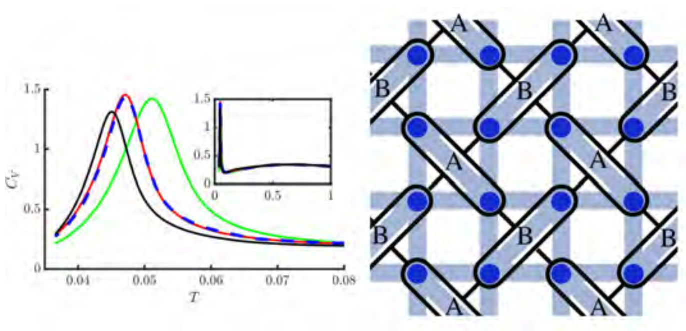
Huerta Alderete, C. Inference-based quantum sensing. . (LA-UR-22-32082)

Huerta Alderete, C., M. E. Hunter Gordon, F. A. Sauvage, A. Sone, A. T. Sornborger, P. J. Coles and M. V. S. Cerezo de la Roca. Inference-based quantum sensing. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22085)

**Peer-reviewed*

Emergent Quantum Phenomena with Tensor Networks

Lukasz Cincio
20190659PRD4



Strong correlations in quantum many body systems result in exotic phases of matter like exotic dimer phases in frustrated magnets (right) and emergent phenomena like phase transitions which can be simulated with tensor networks (left).

Project Description

The development of quantum computers is crucial for the national security. It requires novel materials and insights into the fundamental properties of quantum systems, which frequently require new numerical methods. The goal of this research is to develop such methods and apply them to materials that may open path to noise resilient topological quantum computation and to fundamental limitations on adiabatic quantum computation used by the D-Wave quantum computer.

Technical Outcomes

The project succeeded in developing tensor network methods for thermal properties of strongly correlated systems. The methods were applied to realistic models of strongly correlated magnetic materials and the Hubbard model which are at the forefront of research in a field of strongly correlated condensed matter. Furthermore, the project resulted in a new approach and state-of-the-art methods for error mitigation for gate-based near-term quantum computers.

Publications

Journal Articles

Cincio, L., D. Bultrini, M. E. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith and P. J. Coles. Unifying and benchmarking state-of-the-art quantum error mitigation techniques. Submitted to *Quantum*. (LA-UR-21-27288)

Cincio, L., M. McKerns, A. T. Sornborger and P. J. Czarnik. Improving the efficiency of learning-based error mitigation. Submitted to *arxiv, quantum science and technology*. (LA-UR-22-23390)

*A. A. *. C. P. J. *. C. L. Czarnik, P. *., P. J. Coles, L. Cincio, P. Czarnik and A. Arrasmith. Error mitigation with Clifford quantum-circuit data. 2021. *Quantum*. **5**: 592. (LA-UR-20-23755 DOI: 10.22331/q-2021-11-26-592)

Czarnik, P. J., A. T. Arrasmith, L. Cincio and P. J. Coles. Qubit-efficient exponential suppression of errors. Submitted to *arXiv+PRX Quantum*. (LA-UR-21-21151)

*Czarnik, P., M. M. Rams, P. Corboz and J. Dziarmaga. Tensor network study of the m = 1/2 magnetization plateau in the Shastry-Sutherland model at finite temperature. 2021. *Physical Review B*. **103** (7): 075113. (LA-UR-20-29946 DOI: 10.1103/PhysRevB.103.075113)

Hunter Gordon, M. E., D. Bultrini, P. J. Czarnik, S. J. Wang, M. V. S. Cerezo de la Roca, P. J. Coles and L. Cincio. The battle of clean and dirty qubits in the era of partial error correction. Submitted to *Physical Review X*. (LA-UR-22-24685)

LaRose, R., A. Mari, S. Kaiser, P. J. Kralekas, A. A. Alves, P. J. Czarnik, M. El Mandouh, M. H. Gordon, Y. Hindy, A. Robertson, P. Thakre, N. Shammah and W. J. Zeng. Mitiq: A software package for error mitigation on noisy quantum computers. Submitted to *arXiv*. (LA-UR-21-25925)

Larocca, M., P. J. Czarnik, K. Sharma, G. Muraleedharan, P. J. Coles and M. V. S. Cerezo de la Roca. Diagnosing Barren Plateaus with Tools from Quantum Optimal Control. 2022. *Quantum*. **6**: 824. (LA-UR-21-24973 DOI: 10.22331/q-2022-09-29-824)

*Lowe, A., M. H. Gordon, P. Czarnik, A. Arrasmith, P. J. Coles and L. Cincio. Unified approach to data-driven quantum error mitigation. 2021. *Physical Review Research*. **3** (3): 033098. (LA-UR-20-28845 DOI: 10.1103/PhysRevResearch.3.033098)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, P. J. Czarnik, L. Cincio and P. J. Coles. Effect of barren plateaus on gradient-free optimization. Submitted to *Quantum*. (LA-UR-20-29699)

Sinha, A., M. Rams, P. J. Czarnik and J. Dziarmaga. Finite temperature tensor network study of the Hubbard model on an infinite square lattice. Submitted to *Physical Review Letters*. (LA-UR-22-26026)

Wang, S., P. J. Coles, P. J. Czarnik, A. T. Arrasmith, M. V. S. Cerezo de la Roca and L. Cincio. Can Error Mitigation Improve Trainability of Noisy Variational Quantum Algorithms?. Submitted to *Physical Review X, arxiv.org*. (LA-UR-21-28574)

*Zhang, Y., L. Cincio, C. F. A. Negre, P. Czarnik, P. J. Coles, P. M. Anisimov, S. M. Mniszewski, S. Tretiak and P. A. Dub. Variational quantum eigensolver with reduced circuit complexity. 2022. *npj Quantum Information*. **8** (1): 96. (LA-UR-21-25349 DOI: 10.1038/s41534-022-00599-z)

Reports

Cincio, L. Error mitigation with Clifford quantum-circuit data. Unpublished report. (LA-UR-22-21698)

Presentation Slides

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Czarnik, P. J. Tensor network simulation of two-dimensional strongly correlated systems. Presented at *IonQ seminar*, College Park, Maryland, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-21998)

Czarnik, P. J., A. Lowe, M. H. Gordon, A. T. Arrasmith, P. J. Coles and L. Cincio. Data-driven error mitigation for near-term quantum computers. Presented at *Seminar of Institute of Theoretical Physics of Jagiellonian University, Cracow*, Cracow, Poland, 2020-12-10 - 2020-12-10. (LA-UR-20-30043)

Czarnik, P. J., A. Lowe, M. H. Gordon, A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation for gate-based quantum computers. Presented at *IonQ seminar*, College Park, Maryland, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-22055)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *Quantum Information Processing*, Munich, Germany, 2021-02-01 - 2021-02-05. (LA-UR-21-20721)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *APS March Meeting*, virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22444)

Lowe, A., M. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, P. J. Coles and L. Cincio. Unified Approach to Data Driven Quantum Error Mitigation. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22591)

Posters

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *QuAlg20*, N/A (virtual), United Kingdom, 2020-09-22 - 2020-09-22. (LA-UR-20-27369)

Lowe, A., M. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, P. J. Coles and L. Cincio. Unified approach to data-driven quantum error mitigation. Presented at *Quantum*

Information Processing, Online, New Mexico, United States, 2021-01-01 - 2021-01-05. (LA-UR-21-20496)

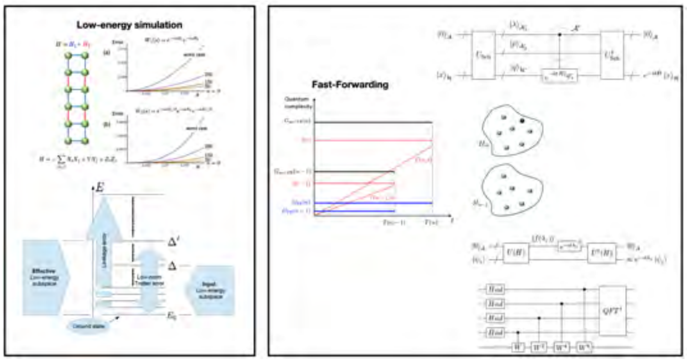
Other

Czarnik, P. J. Data from quantum many-body system calculations. Dataset. (LA-UR-22-21671)

**Peer-reviewed*

Quantum Simulation of Quantum Field Theories

Rolando Somma
20200678PRD1



Left: Dynamical low-energy simulation is more efficient in the low-energy subspace. Right: A general definition of fast-forwarding for quantum systems, and the quantum circuits that fast-forwards the evolution of permutation symmetric Hamiltonians (top) and frustration-free Hamiltonians at low-energies (bottom).

Project Description

This project studies foundational questions on the simulation of quantum field theories (QFTs), which describe the most fundamental particle interactions, with quantum computers. In contrast to standard computers, quantum computers are built upon quantum systems and exploit resources that would not be available otherwise. The expected outcomes are efficient quantum computational methods to study QFTs in regimes that are currently intractable, even for the largest supercomputers. A top quantum algorithms capability is essential for the Department of Energy and National Nuclear Security Administration to succeed in its quest to become world leaders in quantum information science. The results are expected to impact a number of missions including the National Quantum Initiative (NQI). The NQI Act calls for the establishment of a whole-of-Government approach to quantum information science.

Technical Outcomes

This project successfully delivered advanced quantum algorithms to simulate quantum field theories (QFT) regimes that are otherwise intractable. These algorithms were shown to perform (i) efficient and rapidly-converging simulations of subspaces of physical relevance; (ii) quantum speedup evolution with exponential/polynomial fast-forwarding in time; and (iii) simulations of states in thermal equilibrium with exponential reduction in complexity using fluctuation theorems. With these results, significant prior obstacles were overcome, opening avenues to realistic quantum simulations of QFTs.

Publications

Journal Articles

*Gu, S., R. D. Somma and B. Sahinoglu. Fast-forwarding quantum evolution. 2021. *Quantum*. **5**: 577. (LA-UR-20-29591 DOI: 10.22331/q-2021-11-15-577)

*Sahinoglu, B. and R. D. Somma. Hamiltonian simulation in the low-energy subspace. 2021. *npj Quantum Information*. **7** (1): 119. (LA-UR-20-23338 DOI: 10.1038/s41534-021-00451-w)

Sahinoglu, M. B., D. Williamson, N. Bultinck, M. Marien, J. Haegeman, N. Schuch and F. Verstraete. Characterizing Topological Order with Matrix Product Operators. 2021. *Annales Henri Poincaré*. **22** (2): 563-592. (LA-UR-20-29927 DOI: 10.1007/s00023-020-00992-4)

Somma, R. D., G. Muraleedharan, Z. P. Holmes, Y. Subasi and M. B. Sahinoglu. Quantum algorithms from fluctuation theorems: Thermal state preparation. Submitted to *Quantum*. (LA-UR-22-21364)

Reports

Somma, R. D. and M. B. Sahinoglu. Complexity of product formulas in digital adiabatic state transformations. Unpublished report. (LA-UR-21-23267)

Presentation Slides

Sahinoglu, M. B. A tensor network framework for topological phases of quantum matter. Presented at *Mathematical Physics Days 2020*, Istanbul, Turkey, 2020-12-11 - 2020-12-13. (LA-UR-20-30131)

Sahinoglu, M. B. What is quantum information science? and How to be a quantum information scientist?. . (LA-UR-21-20600)

Sahinoglu, M. B. Error correction with tensor networks. Presented at *INT Program 21-1c: Tensor Networks in Many Body and Quantum Field Theory*, Seattle, Washington, United States, 2021-05-17 - 2021-06-04. (LA-UR-21-25022)

Sahinoglu, M. B. Quantum walks - an introduction. . (LA-UR-21-26393)

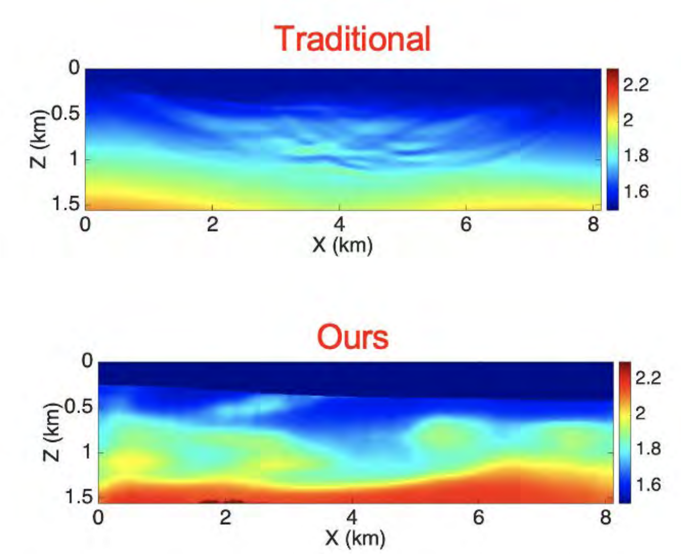
Sahinoglu, M. B. On two pillars of quantum computing: Fault tolerance and Hamiltonian simulation. . (LA-UR-21-27823)

Sahinoglu, M. B. and R. D. Somma. Hamiltonian simulation in the low energy subspace. . (LA-UR-20-27396)

**Peer-reviewed*

Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches

Youzuo Lin
20210542MFR



The comparison of the 2-dimensional imaging results with field data using (top) traditional method and (bottom) our proposed physics-informed data-driven imaging method. This method can characterize the subsurface with much more geologic features.

Project Description

This project will build a capability in physics-informed machine learning, and will be poised for future subsurface energy & security programmatic efforts in carbon dioxide (CO2) sequestration, geothermal extraction, groundwater remediation, and underground nuclear-explosion monitoring, and the national security goal of energy security.

Technical Outcomes

The project team developed InversionNet3D (InvNet3D), an efficient and scalable encoder–decoder network for 3-dimensional full waveform inversion. The method employs group convolution in the encoder to establish an effective hierarchy for learning information from multiple sources while reducing unnecessary parameters and operations at the same time. Experiments on the 3-dimensional Kimberlina dataset demonstrate that InvNet3D achieves state-of-the-art reconstruction performance with lower computational cost and a lower memory footprint compared to the baseline.

Publications

Journal Articles

*Feng, S., X. Zhang, B. Wohlberg, N. P. Symons and Y. Lin. Connect the Dots: In Situ 4-D Seismic Monitoring of CO2 Storage With Spatio-Temporal CNNs. *IEEE Transactions on Geoscience and Remote Sensing*. **60**: 4505216. (LA-UR-21-22295 DOI: 10.1109/TGRS.2021.3116618)

*Feng, S., Y. Lin and B. Wohlberg. Multiscale Data-Driven Seismic Full-Waveform Inversion With Field Data Study. *IEEE Transactions on Geoscience and Remote Sensing*. **60**: 4506114. (LA-UR-21-20004 DOI: 10.1109/TGRS.2021.3114101)

Lin, Y., S. Feng, P. Jin and X. Zhang. Exploring Multi-physics with ExtremelyWeak Supervision. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-22-21115)

Lin, Y., Y. Feng, S. Feng, C. Deng, P. Jin and X. Zhang. OpenFWI: Benchmark Seismic Datasets for Machine Learning-Based Full Waveform Inversion. Submitted to *Geophysical Prospecting*. (LA-UR-21-31188)

Lin, Y., Y. Yang and X. Zhang. Making Invisible Visible: Data-Driven Seismic Inversion with Physics-Driven Data Augmentation. Submitted to *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*. (LA-UR-21-22294)

Lin, Y. and C. Deng. On the Robustness and Generalization of Deep Learning Driven Full Waveform Inversion. Submitted to *SIAM journal on mathematics of data science*. (LA-UR-21-31667)

Lin, Y. and X. Zhang. Spatio-Temporal Graph Convolutional Networks for Earthquake Source Characterization. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-21-20806)

*Zeng, Q., S. Feng, B. Wohlberg and Y. Lin. InversionNet3D: Efficient and Scalable Learning for 3-D Full-Waveform Inversion. *IEEE Transactions on Geoscience and Remote Sensing*. **60**: 1-16. (LA-UR-21-22293 DOI: 10.1109/TGRS.2021.3135354)

Conference Papers

Lin, Y., B. E. Wohlberg and J. P. Theiler. Physics-Consistent Data-driven Seismic Inversion with Adaptive Data Augmentation. Presented at *the 34th Conference on Neural Information Processing Systems (NeurIPS)*. (Vancouver, Canada, 2020-12-06 - 2020-12-06). (LA-UR-20-27731)

Lin, Y., Q. Zeng, S. Feng and B. E. Wohlberg. 3D FullWaveform Inversion via Deep Encoder-Decoder Networks. Presented at *SEG 2021 Annual Meeting*. (denver, Colorado, United States, 2021-09-26 - 2021-09-26). (LA-UR-21-23217)

Lin, Y., Y. Yang and X. Zhang. Enhancing Data-Driven Seismic Inversion using Physics-Guided Spatiotemporal Data Augmentation. Presented at *SEG 2021 Annual Meeting*. (denver, Colorado, United States, 2021-09-26 - 2021-09-26). (LA-UR-21-23216)

Lin, Y. and B. E. Wohlberg. How Good Is Your Scientific Data Generative Model?. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*. (denver, Colorado, United States, 2020-11-15 - 2020-11-15). (LA-UR-20-27518)

Presentation Slides

Feng, S., P. Jin, X. Zhang, Y. Chen, D. Alumbaugh, M. Commer and Y. Lin. Extremely Weak Supervision Inversion of Multi-physical Properties. Presented at *The International Meeting for Applied Geoscience & Energy*, Houston, Texas, United States, 2022-08-27 - 2022-09-01. (LA-UR-22-29088)

Feng, S., X. Zhang, B. E. Wohlberg, N. P. Symons and Y. Lin. Connect the Dots:\xc2\xa0In Situ\xc2\xa04-D Seismic Monitoring of CO2\xc2\xa0Storage With Spatio-Temporal CNNs. . (LA-UR-22-26913)

Lin, Y. Demystifying Career in National Lab. Presented at *Professional Development Seminar at the School of Mathematical and Statistical Sciences, ASU*, tempe, Arizona, United States, 2020-11-16 - 2020-11-16. (LA-UR-20-29376)

Lin, Y. Subsurface Geophysical Imaging. Presented at *LANL-BEG Workshop*, Los Alamos, New Mexico, United States, 2021-04-15 - 2021-04-15. (LA-UR-21-23653)

Lin, Y. Physics-Guided Learning-Driven Computational Seismic Imaging: from Synthetic Practice to Field Applications. Presented at *AAAI Fall Symposium Series (FSS) 2021 - second Symposium on Science-Guided AI (Virtual)*, Los Alamos, New Mexico, United States, 2021-11-04 - 2021-11-06. (LA-UR-21-31071)

Lin, Y. Physics-Informed Data-Driven Seismic Full-Waveform Inversion: from Synthetic Practice to Field Applications. Presented at *SEG Workshop on Data Analytics & Machine Learning for Exploration & Production*, Houston, Texas, United States, 2022-05-16 - 2022-05-19. (LA-UR-22-24544)

Lin, Y. Physics-Guided Data-Driven Seismic Full-Waveform Inversion: Recent Progress on Model Development and Data Sharing. Presented at *2022 SEG/IMAGE Annual Conference*, Houston, Texas, United States, 2022-08-29 - 2022-08-29. (LA-UR-22-29275)

Lin, Y., B. E. Wohlberg, J. P. Theiler and S. Feng. Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches. . (LA-UR-21-22633)

Lin, Y., D. Coblentz, P. A. Johnson, R. J. Pawar, G. D. J. Guthrie, J. P. Theiler, B. E. Wohlberg, S. Feng and Q. Zeng. Physics-Guided Learning-Driven Computational Seismic Imaging: from Synthetic Practice to Field Applications. Presented at *Machine Learning in Solid Earth Geoscience (Online Seminar Series)*, Los Alamos, New Mexico, United States, 2021-09-10 - 2021-09-10. (LA-UR-21-28839)

Lin, Y., S. Feng, P. Jin, B. E. Wohlberg and J. D. Moulton. CycleFCN: A Physics-Informed Data-driven Seismic Waveform Inversion Method. Presented at *SEG Annual Meeting*, Houston, Texas, United States, 2020-10-12 - 2020-10-12. (LA-UR-20-28299)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Monitoring and Forecasting CO2 Storage in the Sleipner area with Spatio-temporal CNNs. Presented at *SEG Annual Conference*, denver, Colorado, United States, 2021-09-26 - 2021-09-26. (LA-UR-21-28468)

Lin, Y., S. Feng and B. E. Wohlberg. InversionNet3D: Efficient and Scalable Learning for 3D Full Waveform Inversion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31917)

Lin, Y., S. Feng and E. Rougier. Machine Learning Tutorial. . (LA-UR-22-27013)

Lin, Y., Y. Yang and B. E. Wohlberg. How Good Is Your Scientific Data Generative Model?. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*, denver, Colorado, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-27918)

Lin, Y., Y. Yang and X. Zhang. Enhancing data-driven seismic inversion using physics-guided spatiotemporal data augmentation. Presented at *SEG Annual Meeting*, denver, Colorado, United States, 2021-09-26 - 2021-09-26. (LA-UR-21-28469)

Lin, Y. and S. Feng. The Application of Unsupervised Physics-informed Full Waveform Inversion on CO2 Monitoring. Presented at *SEG Workshop on Data Analytics & Machine Learning for Exploration & Production*, Houston, Texas, United States, 2022-05-16 - 2022-05-19. (LA-UR-22-24542)

Posters

Lin, Y., C. Deng and S. Feng. Physics semantic Data Augmentation via Disentangled Representation Learning. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-32189)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. 4D Seismic Monitoring and Forecasting of CO2 Sequestration with Neural Networks. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31916)

Lin, Y., S. Feng and B. E. Wohlberg. Style transfer as Data Augmentation for Multiscale Data-driven Full Waveform Inversion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31915)

Lin, Y., Y. Liu and S. Feng. Mitigating data scarcity for joint physics-based and data-driven time-lapse seismic inversion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31785)

Other

Lin, Y. OpenFWI Dataset Documentation. Dataset. (LA-UR-21-30410)

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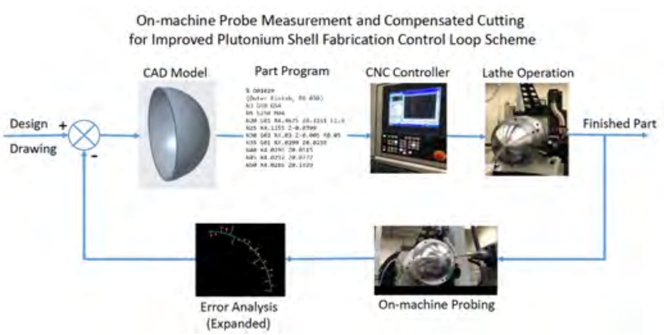
**Peer-reviewed*

On-Machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication

Wendel Brown
20210586MFR



Analogous to a common electrical or mechanical closed loop control system, on-machine measurement and error compensation using a commercially available touch probe, can ensure that more shell components meet their dimensional design requirements. This is the first implementation of this manufacturing technology in support of the Plutonium Pit Production Project. [Image credit: Los Alamos National Laboratory]

Project Description

Precision plutonium shell machining is a key process in the flowsheet for pit manufacturing at the Plutonium Facility at Los Alamos National Laboratory (LANL). The quality of machined shells is assessed against extremely tight specifications for geometric dimensions. Fabrication of these critically important shells has historically been challenging, primarily due to plutonium deforming under dynamic cutting forces from the cutting tool. Other sources of dimensional error can be attributed to temperature fluctuations, operator setup difficulties, and mechanical issues with the machine tool. All of these error sources can be compensated for in the part program, if they can be determined while the shell is mounted on the machine. By measuring points on the surface of the shells and then compensating for dimensional errors, it is expected that a greater than 90 percent product yield can be achieved.

Technical Outcomes

This project was able to successfully demonstrate, for the first time in a plutonium glovebox environment, that on-machine tool and part probing technology can significantly improve shell quality and product yield. Using error compensation techniques for both cutting tool location and tool path generation, shell dimensional conformance is currently achieved on a routine basis. Probe system calibration required algorithm development and played a significant role in the success of this research.

Publications

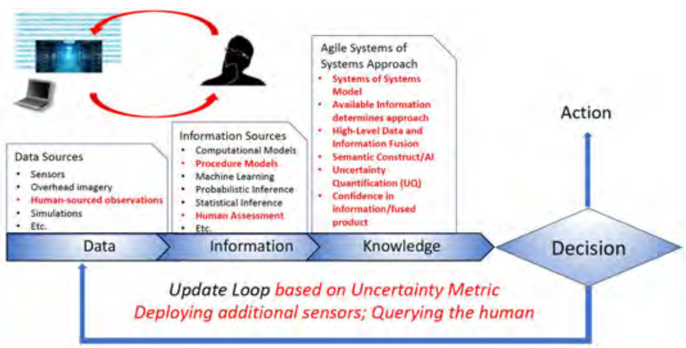
Presentation Slides

Brown, W. G. Mid-year Project Review on 20210586MFR "On-Machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication". . (LA-UR-21-22488)

**Peer-reviewed*

Uncertainty Quantification and Systems of Systems Approach for Robust Decision Support in Strategic Nuclear Deterrence

Kari Sentz
20220799DI



The deterrence problem is analyzed through sets of possible scenarios that are consistent with the available information and develop robust strategies. These are propagated through a systems of systems model that incorporates sensor data, signal processing, physical models/simulations of engineered systems, expert judgement, and statistical machine learning/artificial intelligence. This meta-model is the basis for an interactive tool that learns what is possible from data and where an analyst, subject matter expert, or decision maker can provide expertise and explore scenarios/strategies under different assumptions or informational states. Note that the human is embedded through the full processing arc. Innovation is highlighted in red.

Project Description

The proposed research develops a robust analytical framework to support decision-making for strategic deterrence. From the 2019 Threat Reduction Advisory Committee for the Office of the Secretary of Defense: "current analytic tools are insufficient… to successfully tackle the complex nuclear deterrence challenges they face during the next 25 years". One reason for this insufficiency is the inability of classical methods to capture uncertainty when the available information is vague, ambiguous, or conflicting. Such information is typical in the strategic and tactical deterrence settings. Another reason for this insufficiency is the failure to systematically integrate human-sourced information with data-derived information. The proposed framework will include a modern uncertainty quantification methodology that can capture vague, ambiguous, and conflicting information in a system-of-systems model that includes the human analyst to provide situational awareness and decision support for mission management. Central to achieving this goal is understanding the uncertainty from each source of information. We propose imprecise probabilities to fully characterize the challenging uncertainties typical in multi-sensor target identification. This offers enhanced capabilities for data fusion. We will provide new metrics to inform requirements for more information, whether is from additional sensors, new sensing technologies, or the integration of human-sourced information, judgement, and decision-making.

Publications

Conference Papers

Skau, E. W., C. L. Armstrong, P. M. D. Truong, D. W. Gerts and K. Sentz. Open World Dempster-Shafer using Complementary Sets. Presented at *International Symposium on Imprecise Probabilities: Theories and Applications 2023*. (Oviedo, Spain, 2023-07-11 - 2023-07-14). (LA-UR-23-21683)

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Sentz, K. WELCOME:LANL/University at Buffalo Collaboration. Presented at *LANL/UB Kick Off Meeting*, Los Alamos, New Mexico, United States, 2023-02-08 - 2023-02-08. (LA-UR-23-21375)

Posters

Armstrong, C. L., E. W. Skau, P. M. D. Truong, D. W. Gerts and K. Sentz. Open World Dempster-Shafer Using Complementary Sets. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-22271)

T. Nguyen-Fotiadis, N. T., A. N. Skurikhin and K. Sentz. Comparing Transformer Models and CNN Models for Semantic Segmentation and Damage Evaluation on the xBD Satellite Imagery Dataset. Presented at *Conference on Data Analysis (CoDA)*, SANTA FE, New Mexico, United States, 2023-03-07 - 2023-03-10. (LA-UR-23-22230)

Sentz, K., A. N. Skurikhin and N. Joseph. Vision Transformer based Approach for Post-Flood Damage Assessment. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-02-09. (LA-UR-23-22066)

Skau, E. W., P. M. D. Truong, C. L. Armstrong and K. Sentz. Accelerated Dempster-Shafer using Tensor Decompositions. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe., New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-22183)

**Peer-reviewed*

Modeling and Simulation for Secure and Resilient Communications Networks

Michael Dixon
20220800DI

LANL's modeling and simulation tooling for cryptographic communications over cyber networks will provide functional analyses for multiple, custom mission sets at all scales.

Project Description

We are developing a novel modeling and simulation software that will objectively assess cyber network proposals using advanced cryptographic solutions. The software will simulate models of large cryptographic networks and measure effective security metrics such as network confidentiality, resilience, and robustness. This tooling will enable stakeholders, decision makers, and cyber professionals to test and verify that proposed cryptographic solutions and network architectures can sufficiently meet system requirements before substantial investment needs to be made to engineer those solutions. This will directly benefit the cyber security of Department of Energy (DOE)/National Nuclear Security Administration (NNSA) and Department of Defense (DoD) cyber modernization efforts by providing additional and improved means of assessing and certifying advanced cryptographic and networking technologies.

Publications

Presentation Slides

Dixon, M. J. Supply Chain & Cyber Systems Assurance Using Zero-Knowledge Proofs. . (LA-UR-22-29156)

**Peer-reviewed*

Measuring Network-Based and Physical Vulnerabilities of Complex Bionetworks

Blake Hovde
20220600DI

Identifying and protecting against vulnerabilities associated with genetic data in the bioeconomy and cybersecurity space.

Project Description

Modern Deoxyribonucleic acid (DNA) sequencing instruments represent an extremely powerful tool for generating genetic data towards actionable medical responses, commercial intellectual property in crop science & biomanufacturing, and expanding disease biosurveillance efforts. Security breaches in these instruments represent a real threat to the bioeconomy and overall national security. This project will work to characterize potential risks in sequencing equipment, misconfigurations in equipment setup and provide mitigation guidance to users of this equipment. This topic falls within a new category of research and development called 'cyberbiosecurity', which encompases protection of the growing global bioeconomy and protected biological data and intellectual property in biological research and development.

Technical Outcomes

Through the use of institutional software tools, commercial off the shelf (COTS) software and hardware security toolsets we focused on investigation of data collection at multiple levels. Queries included local hardware vulnerabilities, intercept of data transfer from the instrument to a local server, intercept of data transfer to a networked server, intercept of sequencing data being transferred to a cloud-based system, or data transfer implementing file transfer protocol (FTP).

Publications

Presentation Slides

Hovde, B. An introduction to Digital Biosecurity/Cyber-Biosecurity. Presented at *SoCalHub Workshop on Secure Autonomy*, Riverside, California, United States, 2022-06-02 - 2022-06-02. (LA-UR-22-25129)

Hovde, B. Introducing Concepts in Digital Biosecurity. Presented at *Gordon Research Conference (GRC) - Bio/Chem Defense*, Ventura, California, United States, 2023-03-19 - 2023-03-24. (LA-UR-23-22944)

Posters

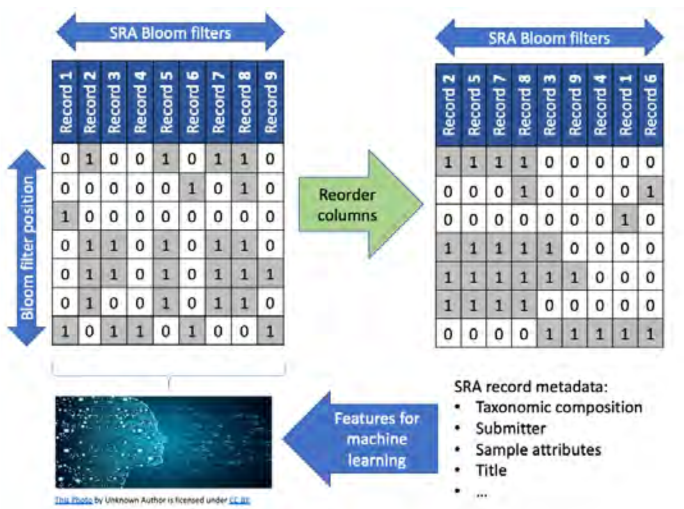
Hovde, B. and A. O. McGuinness. CRISPR Off-target Damage Analysis. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27610)

**Peer-reviewed*

Safeguarding the Integrity of the Sequence Read Archive

Jason Gans

20220602DI



The proposed database of Bloom filters represents deoxyribonucleic acid (DNA) sequences as columns of bits and stores multiple Bloom filters as a matrix of bits. Bloom filter bit matrices can be efficiently compressed by reordering the columns to creates contiguous runs of 1's and 0's. Since there are too many sequence records to precompute and store all of the corresponding Bloom filters, it is essential to computationally predict which sequence records are likely to yield similar Bloom filters. This project will develop a machine learning algorithm to predict sequence records likely to produce similar, compressible, Bloom filters using sequence record metadata.

Project Description

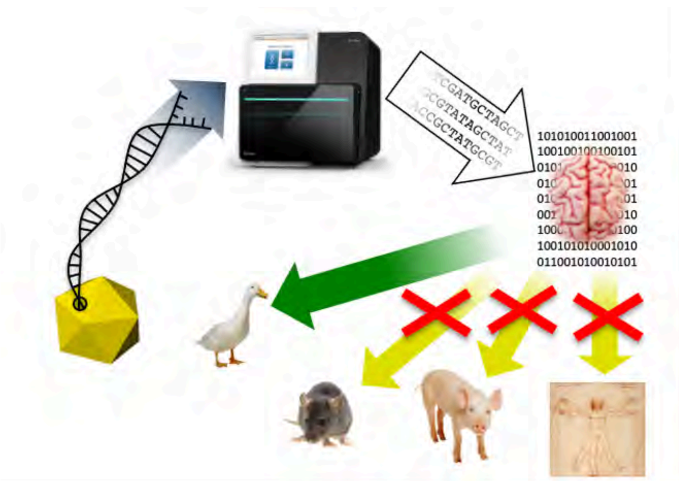
At approximately fifteen petabytes and doubling every 26 months, the Sequence Read Archive (SRA) is the largest repository of biological sequence data in the world. Reflecting the diversity of modern genomic science, the SRA is an invaluable data trove of sequences from diverse sample types, including the coronavirus (Covid-19) pandemic, clinical and environmental microbial communities, and gene expression studies. In addition, the SRA also contains information that can reveal unpublished activities occurring in laboratories around the world. This information "leakage" is a result of laboratory contamination that can occur prior to the sequencing of biological samples. This effort will help safeguard the integrity of the SRA by enabling the creation of a compact database of "thumbnail sketches" representing individual SRA records. The "thumbnail sketch" of each record will be implemented with Bloom filter data structures, which provide lossy compression via a trade-off between storage size and the probability of reporting a false positive. Unlike simple checksums, which only determine if a record has been modified, the Bloom filter representation supports sequence-based searches that can provide information on the potential sequence differences. By storing the SRA sketches on local computer systems, changes to the primary SRA database can be detected and characterized.

Technical Outcomes

Improvements in algorithm speed, reliability, and compression provide the groundwork for follow on work to build a compact, searchable version of the Sequence Read Archive (SRA). The feasibility analysis shows that a 100-fold reduction in storage space is likely out of reach for a Bloom filter SRA database. However, 50-fold reduction in size is definitely feasible.

Predicting Viral Phenotype from Genotype

Jason Gans
20220610DI



Even though viral genome sequences are routinely sequenced and assembled, inferring important information about a virus, like the reservoir host, can be very difficult. To address this challenge and close the "measurement-to-inference" loop, this project will implement and evaluate machine learning algorithms to computationally predict viral properties from sequenced viral genomes.

Project Description

A significant fraction of viruses known to infect humans originated in wild animals, and new viruses continue to spill over into the human population. Recent outbreaks of ebolavirus in West Africa and the ongoing Severe Acute Respiratory Syndrome-Coronavavirus 2 (SARS-CoV-2) pandemic demonstrate the need for rapid and reliable characterizations of viruses to help control disease spread. In particular, knowledge of the reservoir host could help answer forensic questions about the start of disease outbreaks and inform control measures to help avoid future outbreaks. Understanding the transmission mode could directly guide appropriate control measures to limit spread of a new virus in the human population. To help address these questions, we propose to develop a machine learning approach to predict the properties of a novel virus from its genome sequence. This approach will test the fundamental assumption that biological constraints on viral genome sequences imposed by viral adaptation to host cellular machinery can be identified and exploited by machine learning. The ability to accurately predict biological phenotype from genotype is a grand challenge problem in computational biology, and progress towards this goal will provide a powerful analysis capability for both open biology and national security research at Los Alamos National Laboratory.

Technical Outcomes

The performance of the developed viral host prediction methods did not reach the level of prediction the project team had been hoping for. However, useful methods for grouping and processing GenBank (an online genome database) records were developed. The probabilistic method created for predicting SARS-CoV-2 genome sequence evolution is an exciting development with potential direct application to improving existing pathogen detection efforts at Los Alamos.

Information Science and Technology Institute (ISTI): Foundational Research in Information Science and Technology

James Ahrens
20210529CR-IST

The ISTI Rapid Response program funds the exploration of new ideas, feasibility studies, or basic R&D in support of upcoming proposal opportunities. The ISTI Rapid Response program accepts proposals in the areas of computational and computer science, quantum computing, and data science.

Project Description

This Information, Science and Technology (IS&T) project addresses national security challenges in the Department of Energy/National Nuclear Security Administration (DOE/NNSA) Defense Program mission space. Maintaining the stockpile requires the simulation of materials under extreme conditions. Goals of this proposal include supporting a collection of IS&T projects that explore using either artificial intelligence, quantum computing or configurable hardware to create faster, higher-fidelity simulations. Another goal focuses on understanding and validating these simulations using advanced data science methods. This proposal also contributes to the DOE/NNSA Nuclear Nonproliferation mission. This mission is to prevent actors from developing nuclear weapons or acquiring weapons-usable nuclear or radiological materials, equipment, technology, and expertise. Achieving this mission requires use of data and methods to detect these activities. To be successful, a final goal is to develop methods that ensure our data and methods are of the highest integrity and have not been manipulated in any way. The expected result of this proposal is to create a collection of high-risk, high-rewards IS&T projects that addresses Los Alamos National Laboratory mission needs. These projects will support workforce development by funding students, post-doctoral scholars and staff.

Publications

Journal Articles

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Jones, S. M., H. R. Jayanetti, A. Osborne, P. Koerbin, M. Klein, M. C. Weigle and M. L. Nelson. The DSA Toolkit Shines Light Into Dark and Stormy Archives. 2022. *code{4}lib Journal*. **53**: 16441. (LA-UR-22-23608)

Jones, S. M., M. Klein, M. Weigle and M. Nelson. Shining a Light into Dark and Stormy Archives through Social Media Storytelling. Submitted to *ACM Transactions on the Web*. (LA-UR-22-27949)

Karra, S., B. Ahmmed and M. Mudunuru. AdjointNet: Constraining machine learning models with physics-based codes. Submitted to *Journal of Computational Physics*. (LA-UR-21-28763)

Savage, D. J., L. Lutterotti, C. M. Biwer, M. McKerns, C. A. Bolme, M. Knezevic and S. C. Vogel. MILK: a python scripting interface to MAUD for automation of Rietveld analysis. Submitted to *Journal of Applied Crystallography*. (LA-UR-22-32248)

Solander, K. C., C. J. Talsma and V. V. (. Vesselinov. The drivers and predictability of wildfire re-burns in the western United States (US). 2023. *Environmental Research: Climate*. **2** (1): 015001. (LA-UR-22-27394 DOI: 10.1088/2752-5295/acb079)

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Yoon, B., C. C. Chang, G. T. Kenyon, N. T. Nguyen and E. Rrapaj. Prediction and compression of lattice QCD data using machine learning algorithms on quantum annealer. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-31665 DOI: 10.22323/1.396.0143)

Conference Papers

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Huang, C., O. Beznosov, Q. Tang, J. W. Burby, A. Kim, H. N. Rakotoarivelo, B. Shen, J. Domine, B. E. Carlsten, G. A. Dilts, R. V. Garimella, T. J. T. Kwan, R. W. Robey and F. Li. Modeling of Nonlinear Beam Dynamics via a Novel Particle-Mesh Method and Surrogate Models With Symplectic Neural Networks. Presented at *North American Particle Accelerator Conference 2022*. (Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12). (LA-UR-22-27745)

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Dixon, M. J., Z. L. DeStefano and D. A. Barrack. zkQMC: Non-Interactive Zero-Knowledge Uncertainty Quantification Using Quasi-Randomness. Unpublished report. (LA-UR-22-23274)

Presentation Slides

Ahrens, J. P. Information Science and Technology Institute Rapid Response R&D and Institutional Program Development programs – Round 1 & 2. . (LA-UR-21-21664)

Beznosov, O. Spin matching and Monte-Carlo simulation of radiative depolarization in electron-positron storage rings with Bmad and SLICKTRACK. Presented at *65th*

ICFA Advanced Beam Dynamics Workshop on High Luminosity Circular e+e- Colliders (eeFACT2022), Rome, Italy, 2022-09-12 - 2022-09-16. (LA-UR-22-29531)

Brady, P. T., D. Livescu and N. Sharan. AI Enhanced Discretizations for High-Fidelity Physics Simulations. . (LA-UR-21-29077)

Caravelli, F. Dynamical systems embeddings and optimization. . (LA-UR-22-29549)

Carpenter, M. H., E. S. Teti and S. Salazar Escobedo. Machine Learning for Hyperspectral X-ray Imaging Analysis. . (LA-UR-21-28927)

Castorena, J. E. Boosting Deep Semi-Supervised Learning with Multi-view Redundant Information. . (LA-UR-21-28998)

Castro, L. A. and N. K. Parikh. Towards a Machine Learning Decision Framework for Streamlining Dengue Virus Forecasting. . (LA-UR-22-29470)

DeStefano, Z. L. Distributed and Verifiable Uncertainty Quantification Using Zero Knowledge Proofs. . (LA-UR-21-26797)

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W. Drobina, E. C., E. A. Moore, M. J. Grosskopf and C. X. Ren. Explaining the Explanation: In Search of Understanding for Saliency Maps. . (LA-UR-22-28547)

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Jayanetti, H., S. M. Jones, M. Klein, A. Osbourne, P. Koerbin, M. L. Nelson and M. C. Weigle. Creating Structure in Web Archives With Collections: Different Concepts From Web Archivists. Presented at *The 26th International Conference on Theory and Practice of Digital Libraries*, Padua, Italy, 2022-09-20 - 2022-09-23. (LA-UR-22-29413)

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Jayawardena, G., B. J. Cain, M. Klein and S. M. Jones. PDF Server: Extracting Metadata from Scientific PDF Documents. Presented at *Mini Summer Student Symposium 2022*, Los Alamos, New Mexico, United States, 2022-08-25 - 2022-08-25. (LA-UR-22-29460)

Jones, S. M. DisrupTECH Application: Exploring Collections By Selecting Exemplars. Presented at *DisrupTECH Application Lighting Talks*, Los Alamos, New Mexico, United States, 2023-03-15 - 2023-03-15. (LA-UR-23-22405)

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Koglin, J. E., J. E. Coleman, M. McKerns, H. E. Morris, N. B. Ramey, A. Scheinker, E. H. Toler and A. B. Williams. Unwrapping radiograph target disassembly using adaptive machine learning. . (LA-UR-22-29529)

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Moore, E. A. Buyer Beware: Unexpected Behaviors of XAI Techniques. . (LA-UR-22-28625)

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Posters

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Huang, C., O. Beznosov, J. W. Burby, B. E. Carlsten, G. A. Dilts, J. Domine, R. V. Garimella, A. Kim, T. J. T. Kwan, H. N. Rakotoarivelo, R. W. Robey, B. Shen, Q. Tang and F. Li. Modeling of Nonlinear Beam Dynamics via A Novel Particle-Mesh Method and Surrogate Models with Symplectic Neural Networks. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-28113)

Jones, S. M. and A. C. Nwala. Revisiting Top News Stories Before 2000 May Be Challenging With Web Archives. Presented at *ACM/IEEE Joint Conference On Digital Libraries*, Santa Fe, New Mexico, United States, 2023-06-26 - 2023-06-30. (LA-UR-23-21898)

Koglin, J. E., J. E. Coleman, M. McKerns, D. Ronquillo and A. Scheinker. Progress toward improving accelerator performance and automating operations with advanced analysis software. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-08 - 2022-08-12. (LA-UR-22-27302)

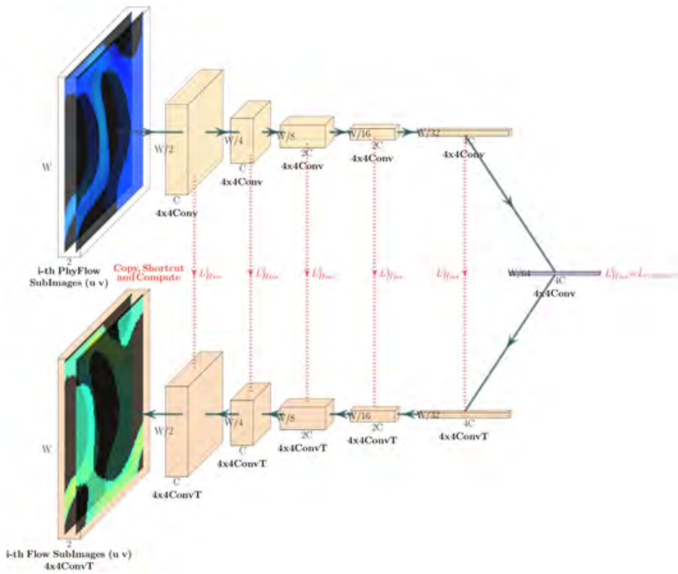
Teti, E. S. and M. H. Carpenter. Data-Driven Automatic Calibration (DDAC) Routine for High-Energy-Resolution X-ray Emission Spectroscopy. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-21974)

Toler, E. H., J. E. Coleman, J. E. Koglin, M. McKerns, H. E. Morris, A. Scheinker and A. B. Williams. Unwrapping Image Data Using Adaptive Machine Learning. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-27123)

**Peer-reviewed*

Modeling Systems out of Equilibrium

Christopher Fryer
20220545CR-CNL



The Convolutional Encoder-Decoder (CED) network architecture for predicting fluid flow in nano-pores of shale formation. The model contains an encoder (upper row), a decoder (bottom row), and a bottleneck in between (middle right). They are composed of consecutive convolutional neural network (CNN) layers. The input images into the model are pore-fluid flow velocity fields simulated from CNN layers implementing the finite difference solutions of classical Navier-Stokes equations. The CED model is physically informed by these images and then learning to output ground-truth nano-pore-fluid fields given by molecular dynamics. Figure from Wang, et al. (2021). J. Computational Physics, 110526.

Project Description

This project addresses the development of computational methods to study the dynamics of fluid and materials out of equilibrium. We will use modern artificial intelligence methods to generate models of flows and granular materials. The results are relevant for fluid dynamics, ocean dynamics, and high explosives. At the most fundamental level, we will develop and investigate new computational methods to study a range of fluid instabilities, turbulent flows, magnetohydrodynamics, and the deformation of materials. We will develop and implement physics-inspired deep learning methods to develop new ways of solving partial differential equations relevant to fluid dynamics and plastic deformations of materials.

We will focus on applications to multi-scale physics relevant to weapon physics, turbulence modeling in ocean and subsurface flows, high explosives, magnetohydrodynamics, and space weather.

Publications

Journal Articles

Barker, B. L., E. O'Connor and S. Couch. Inferring Type II-P Supernova Progenitor Masses from Plateau Luminosities. 2023. *The Astrophysical Journal Letters*. **944** (1): L2. (LA-UR-22-31879 DOI: 10.3847/2041-8213/acb052)

Chen, R., T. R. Gibson and G. T. Craven. Energy transport between heat baths with oscillating temperatures. Submitted to *Physical Review E*. (LA-UR-23-22404)

Holmbeck, E. M., J. Barnes, K. A. Lund, T. M. Sprouse, G. C. McLaughlin and M. R. Mumpower. Superheavy Elements in Kilonovae. Submitted to *Astrophysical Journal Letters*. (LA-UR-23-23123)

Jayakumar, A., M. D. Vuffray and A. Lokhov. Learning Energy Based Representations of Quantum Many-Body States. Submitted to *Nature Physics*. (LA-UR-23-23196)

Leone, L., S. Oliviero, A. Hamma and S. Lloyd. Black Hole complexity, unscrambling, and stabilizer thermal machines. Submitted to *Physical Review Letters*. (LA-UR-22-33044)

Liu, L., J. A. Estrada Santos, M. Prodanovic and M. Pyrcz. Mitigation of Spatial Nonstationarity with Vision Transformers. Submitted to *Computers & Geosciences*. (LA-UR-22-32653)

Lund, K. A., J. Engel, G. C. McLaughlin, M. R. Mumpower, E. M. Ney and R. Surman. The Influence of \xce\xb2-decay Rates on r-process Observables. 2023. *The Astrophysical Journal*. **944** (2): 144. (LA-UR-22-28160 DOI: 10.3847/1538-4357/acaf56)

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Pachalieva, A. A., M. R. Sweeney, H. S. Viswanathan, E. Stein, R. Leone and J. D. Hyman. Impact of artificial topological changes on flow and transport through fractured media due to mesh resolution. Submitted to *Computational Geosciences*. (LA-UR-23-20307)

Pachalieva, A. A., R. S. Pavel, J. A. Estrada Santos, A. Diaw, N. E. Lubbers, J. R. Haack, C. Junghans, D. Livescu, T. C. Germann and H. S. Viswanathan. GLUE Code: A framework handling communication and interfaces between scales. 2022. *Journal of Open Source Software*. **7** (80): 4822. (LA-UR-22-29746 DOI: 10.21105/joss.04822)

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Prodanovic, M., M. Esteva, J. McClure, B. Chang, J. A. Estrada Santos, A. Radhakrishnan, A. Singh and H. Khan. Digital Rocks Portal(Digital Porous Media): connecting data, simulation and community. Submitted to *Society of Core Analysts*. (LA-UR-22-24710)

S. Cerezo de la Roca, M. V., L. Leone, S. Oliviero and L. Cincio. On the practical usefulness of the Hardware Efficient Ansatz. Submitted to *Quantum Science and Technology*. (LA-UR-22-31539)

Saccone, M. D., A. Van den Berg, E. Harding, S. Singh, S. R. Giblin, F. Flicker and S. Ladak. Exploring the phases of 3D artificial spin ice: From Coulomb phase to magnetic monopole crystal. Submitted to *Nature Physics*. (LA-UR-22-32126)

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*Sadler, J. D., C. A. Walsh, Y. Zhou and H. Li. Role of self-generated magnetic fields in the inertial fusion ignition threshold. 2022. *Physics of Plasmas*. **29** (7): 072701. (LA-UR-21-30942 DOI: 10.1063/5.0091529)

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Estrada Santos, J. A., B. Chang, A. Gigliotti, Y. Yin, W. Song, M. Prodanovic, Q. Kang, N. E. Lubbers and H. S. Viswanathan. DRP-372: A Dataset of 3D Structural and Simulated Transport Properties of Complex Porous Media. Submitted to *Nature Scientific Datasets*. (LA-UR-22-24711)

Estrada Santos, J. A., Z. Fox, A. T. Mohan, H. S. Viswanathan and N. E. Lubbers. The Senseiver: attention-based global field reconstruction from sparse observations. Submitted to *nature machine intelligence*. (LA-UR-22-31480)

*Santos, J. E., A. Gigliotti, A. Bihani, C. Landry, M. A. Hesse, M. J. Pyrcz and M. Prodanovi\xc4\x87. MPLBM-UT: Multiphase LBM library for permeable media analysis. 2022. *SoftwareX*. **18**: 101097. (LA-UR-22-23120 DOI: 10.1016/j.softx.2022.101097)

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Shastry, A., A. Jayakumar, C. Bhattacharyya and A. Patel. Reliable Quantum Kernel Classification using fewer Circuit Evaluations. Submitted to *Physical Review X*. (LA-UR-22-28394)

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Wang, K. and K. Bennett. Learning particle physics simulations with physics-informed convolutional encoder-decoders. Submitted to *Journal of Computational Physics*. (LA-UR-22-29244)

Weijer, W., T. Haine, A. Siddiqui, W. Cheng, C. Veneziani and P. K. Kurtakoti. Interactions between the Arctic Mediterranean and the Atlantic Meridional Overturning Circulation: A Review. 2022. *Oceanography*. **35** (3-4): 130. (LA-UR-22-27688 DOI: 10.5670/oceanog.2022.130)

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Chang, B., J. A. Estrada Santos, R. Victor, H. S. Viswanathan and M. Prodanovic. Improving Machine Learning Predictions of Rock Electric Properties Using 3D Geometric Features. Presented at *SPE Annual Technical Conference and Exhibition*. (Houston, Texas, United States, 2022-10-03 - 2022-10-05). (LA-UR-22-26767)

Chang, B., J. A. Estrada Santos, R. Victor and M. Prodanovic. ElRock-Net: Assessing the Utility of Machine Learning to Initialize 3D Electric Potential Simulations. Presented at *Society of Core Analysts*. (Austin, Texas, United States, 2022-09-19 - 2022-09-22). (LA-UR-22-29665)

Jayakumar, A., M. D. Vuffray and A. Lokhov. Energy based models for tomography of quantum spin-lattice systems. Presented at *Machine Learning and the Physical Sciences*. (New Orleans, Louisiana, United States, 2022-12-03 - 2022-12-03). (LA-UR-22-30151)

Estrada Santos, J. A., Z. Fox, A. T. Mohan, H. S. Viswanathan and N. E. Lubbers. The Senseiver: attention-based global field reconstruction from sparse observations. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*. (New Orleans, Louisiana, United States, 2022-11-28 - 2022-12-09). (LA-UR-22-30098)

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Capodaglio, G., M. R. Petersen, A. K. Turner and A. F. Roberts. An unstructured C-grid type variational formulation for the sea ice dynamics. Unpublished report. (LA-UR-21-32250)

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Chen, R., G. T. Craven and T. R. Gibson. Controlling molecular heat conduction using temperature modulations. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-21317)

Lund, K. A. Kilonova Modeling. Presented at *N3AS Summer School in Multi-Messenger Astrophysics*, Santa Cruz, California, United States, 2022-07-31 - 2022-08-07. (LA-UR-22-27785)

Lund, K. A. Magnetic Fields in Kilonova Modeling. Presented at *T-Division Student Lightning Talks*, Los Alamos, New Mexico, United States, 2022-08-10 - 2022-08-10. (LA-UR-22-28172)

Lund, K. A. Kilonova Modelling: Nuclear Physics, Magnetic Fields, Neutrinos. Presented at *International School of Nuclear Physics 43rd Course Neutrinos in Cosmology, Astro-, Particle- and Nuclear Physics*, Erice, Italy, 2022-09-17 - 2022-09-17. (LA-UR-22-29804)

Lund, K. A. Key Uncertainties in Astrophysical r-Process Nucleosynthesis. Presented at *Remnants of neutron-star mergers - Connecting hydrodynamics models to nuclear, neutrino, and kilonova physics*, Darmstadt, Germany, 2022-10-17 - 2022-10-20. (LA-UR-22-30999)

Lund, K. A., Y. Zhu, J. Barnes, T. M. Sprouse, N. Vassh, G. McLaughlin, M. R. Mumpower and R. Surman. Probing Nuclear Uncertainties in Kilonova Modeling. Presented at *15th International Conference on Nuclear Data for Science and Technology*, Sacramento, California, United States, 2022-07-21 - 2022-07-29. (LA-UR-22-27145)

Pang, Y., A. Jayakumar, E. McKinney, C. J. Coffrin, M. D. Vuffray and A. Lokhov. Unreasonable effectiveness of pairwise Markov random fields in finding ground states of stoquastic Hamiltonians. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22280)

Saccone, M. D. and F. Caravelli. How nanomagnets process information. Presented at *MMM 2022*, Minneapolis, Minnesota, United States, 2022-10-31 - 2022-10-31. (LA-UR-22-31280)

Schimming, C. D. Active Nematics in Geometric Confinement. Presented at *CNLS Postdoc Seminar*, Los Alamos, New Mexico, United States, 2023-03-23 - 2023-03-23. (LA-UR-23-23056)

Schimming, C. D., C. J. Reichhardt and C. Reichhardt. Friction mediated transition to boundary dependent bidirectional flows in circularly confined active nematics. Presented at *Active Matter in Complex Environments*, Aspen, Colorado, United States, 2023-01-01 - 2023-01-06. (LA-UR-22-33122)

Schimming, C. D. and J. Vinals. Analytical predictions for 3D disclination motion. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22169)

Tovar, E. J. Robust second-order approximation of the compressible Euler equations with an arbitrary equation of state. Presented at *International Conference on Numerical Methods for Multi-Material Fluid Flow (MultiMat)*, Zurich, Switzerland, 2022-08-22 - 2022-08-26. (LA-UR-22-28744)

Tovar, E. J. A high-order explicit Runge-Kutta method for approximating the Shallow Water Equations with sources. Presented at *5th Annual Meeting of the SIAM Texas-Louisiana Section*, Houston, Texas, United States, 2022-11-04 - 2022-11-06. (LA-UR-22-31706)

Wang, K., C. W. Johnson, K. Bennett and P. A. Johnson. Predicting the Future Fault Frictional Coefficient in a Shear Experiment Applying Deep Learning. Presented at *AGU 2021 Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31894)

Weijer, W., Y. Li, P. K. Kurtakoti, C. Veneziani and P. Chang. Distinct Responses of the Arctic Atmosphere to Pacific and Atlantic Ocean Heat Transport. Presented at *High-resolution modelling workshop*, College Station, Texas, United States, 2023-01-23 - 2023-01-25. (LA-UR-23-20575)

Posters

Jayakumar, A., M. D. Vuffray and A. Lokhov. Energy based models for tomography of quantum spin-lattice systems. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*, New Orleans, Louisiana, United States, 2022-11-28 - 2022-12-03. (LA-UR-22-32410)

Estrada Santos, J. A., A. Marcato, G. Boccardo, H. S. Viswanathan, D. Marchisio and M. Prodanovic. Prediction of Concentration Fields in Porous Media Using a Multiscale Neural Network. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32655)

Schimming, C. D. Friction mediated transition to boundary dependent bidirectional flows in circularly confined active nematics. Presented at *Active Matter in Complex Environments*, Aspen, Colorado, United States, 2023-01-01 - 2023-01-06. (LA-UR-22-32892)

Weijer, W., S. V. S. Brand, C. Veneziani, Z. Kaufman and P. K. Kurtakoti. Ocean and Atmosphere Heat Transport Anomalies linked to Weddell Sea Polynyas. Presented at *Ocean Sciences Meeting*, Honolulu, Hawaii, United States, 2022-02-24 - 2022-03-04. (LA-UR-22-21238)

Younas, N. Building a Quantum computer using a molecular spins.. . (LA-UR-22-27636)

**Peer-reviewed*

Machine Learning Enhanced Modeling

Enrique Batista
20200001CR-CNL

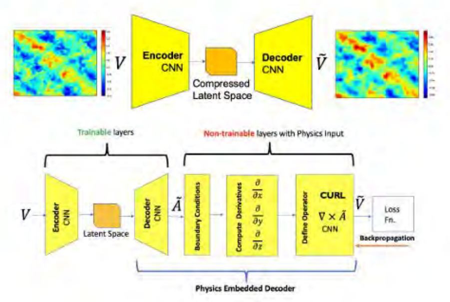

Illustration of the physics inspired machine learning methodology developed to embed hard physical constraints in neural network coarse-graining of 3D (3-dimensional) turbulence. The top image shows the standard, physics-agnostic Convolutional Auto Encoder (CAE) architecture, with the 3D velocity field training dataset as input V (velocity field). The challenge is to embed physical constraints to ensure that the CAE only learns a latent space such that it satisfies physical constraints. The bottom figure shows the physics-embedded Auto Encoder (PhyCAE), which imposes non-trainable constraints that describe boundary conditions and other conserved quantities when optimizing the network.

Project Description

This project will develop tools that merge optimization theory, cutting-edge computational and algorithmic machine learning methods, with physical knowledge in the form of constraints, symmetries, and domain expertise regarding effective degrees of freedom. Our focus is to develop methodologies for automated model reduction and coarsening, learning macro-scale and atomistic models that capture relevant physics of micro-scale simulations, and algorithms for the optimization and control of power and infrastructure systems. The resulting technologies are applicable to a wide range of problems in chemistry, materials, biological systems, power grid modeling, and fluid dynamics. The research is done in interdisciplinary teams that include engineers, physicists, chemists, and mathematicians. Postdoctoral fellows conduct the research under the supervision of Laboratory staff scientists. The project will explore frontiers areas of research that are relevant to the Laboratory programs and missions. This work is also in perfect alignment with the Department of Energy (DOE) Office of Science “Artificial Intelligence (AI) for Science” initiative.

Technical Outcomes

This project developed approaches to leverage physical knowledge to improve the performance of modern machine learning methods, and develop novel numerical methods to solve challenging optimization problems.

Publications

Journal Articles

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*Nunes, F. M., T. Poxon-Pearson, M. Catacora-Rios, L. Hlophe, J. Pereira, G. B. King, A. E. Lovell and G. Potel. Extracting capture from transfer reactions. 2020. *Journal of Physics: Conference Series*. **1668**: 012030. (LA-UR-19-31196 DOI: 10.1088/1742-6596/1668/1/012030)

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Quantum Mechanics.. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-30735)

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Geth, F., C. J. Coffrin and D. M. Fobes. A Flexible Storage Model for Power Network Optimization. Presented at *1st International Workshop on Challenges and Opportunities in the Design and Operation of Energy Storage Systems*. (Melbourne, Australia, 2020-06-26 - 2020-06-26). (LA-UR-19-29733)

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Rupe, A. T., V. V. Vesselinov, B. T. Nadiga, D. F. DeSantis and M. Anghel. Transfer Operator Framework for Earth System Predictability and Water Cycle Extremes. Unpublished report. (LA-UR-21-22681)

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Kannan, R., N. Ho-Nguyen and J. R. Luedtke. Data-Driven Multi-Stage Stochastic Optimization on Time Series. Presented at *The seventh International Conference on Continuous Optimization (ICCOPT)*, Bethlehem, Pennsylvania, United States, 2022-07-28 - 2022-07-28. (LA-UR-22-27528)

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Lovell, A. E. Uncertainty Quantification for Reaction Theory. . (LA-UR-20-23038)

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Lovell, A. E., A. T. Mohan and P. Talou. Probabilistic Machine Learning for Uncertainty Quantification. Presented at *Machine Learning for Nuclear Data*, Online, New Mexico, United States, 2020-12-08 - 2020-12-08. (LA-UR-20-29925)

Molnar, J. P. Applied Scientific Machine Learning for Parameter Estimation. Presented at *T Division Lightning Talks*, Los Alamos, New Mexico, United States, 2022-07-27 - 2022-07-27. (LA-UR-22-27461)

Rupe, A. T. Ergodic Theory and Dynamical Process Modeling. . (LA-UR-21-20546)

Rupe, A. T. Learning Implicit Models of Complex Dynamical Systems From Partial Observations. . (LA-UR-21-26946)

Rupe, A. T. The Search For Thermodynamic Principles of Organization. . (LA-UR-21-27304)

Rupe, A. T. PNNL Technical Interview. . (LA-UR-22-25759)

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Teti, M. A. CNNs With a Neuromorphic Sparse Coding Frontend are More Robust to Adversarial Attacks. Presented at *Naval Applications of Machine Learning (NAML)*, Virtual, California, United States, 2022-03-22 - 2022-03-24. (LA-UR-22-21808)

Teti, M. A. CNNs With a Neuromorphic Sparse Coding Frontend are More Robust to Adversarial Attacks. Presented at *Naval Applications of Machine Learning (NAML)*, Virtual, California, United States, 2022-03-22 - 2022-03-24. (LA-UR-22-22116)

Weisser, T. Recover Functional Relations from Moment Information. Presented at *Arizona Days*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-18. (LA-UR-20-23852)

Yang, H. and H. Nagarajan. Distribution Network Optimization under Stochastic Disruptions. Presented at *INFORMS Annual Meeting 2020*, Online, New Mexico, United States, 2020-11-07 - 2020-11-13. (LA-UR-20-28337)

Yang, H. and H. Nagarajan. Distribution Network Optimization Under Stochastic Disruptions. Presented at *INFORMS Annual Meeting 2020*, Online, New Mexico, United States, 2020-11-07 - 2020-11-13. (LA-UR-20-28580)

Zhou, G., N. E. Lubbers, K. M. Barros, B. T. Nebgen and S. Tretiak. Machine Learning with Domain Knowledge in Quantum Chemistry. Presented at *Telluride Workshop "Machine Learning and Informatics for Chemistry and Materials"*, Telluride, Colorado, United States, 2021-09-27 - 2021-10-01. (LA-UR-21-29365)

Posters

Goutham, M., R. Kannan, D. Deka, H. Nagarajan and R. W. Bent. Optimal Power Flow for Resilient Electric Grids under Uncertain Hurricane Forecasts: A Multi-Stage Stochastic Programming Approach. Presented at *2023 Grid Science Winter School and Conference*, Santa Fe, New Mexico, United States, 2023-01-09 - 2023-01-13. (LA-UR-23-20059)

Moraru, M., M. Warnet, J. Loiseau, V. B. Ramakrishnaiah, N. A. Prajapati, H. Lim, R. S. Pavel, S. Lakshmiranganatha, J. Mohd-Yusof, A. R. Reisner, K. C. Tsai, R. F. Berger and P. S. McCormick. Transformations for Energy Efficient Accelerated Chain Matrix Multiplication (TEE-ACM2). Presented at *LANL Student Symposium 2022*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27515)

Moraru, M., M. Warnet, J. Loiseau, V. B. Ramakrishnaiah, N. A. Prajapati, H. Lim, S. Lakshmiranganatha, J. Mohd-Yusof, K. C. Tsai, R. F. Berger and P. S. McCormick. Transformations for Energy Efficient Accelerated Chain Matrix Multiplication (TEE-ACM2). Presented at *Supercomputing - The International Conference for High Performance Computing, Networking, Storage and Analysis*, Dallas, Texas, United States, 2022-11-13 - 2022-11-18. (LA-UR-22-28472)

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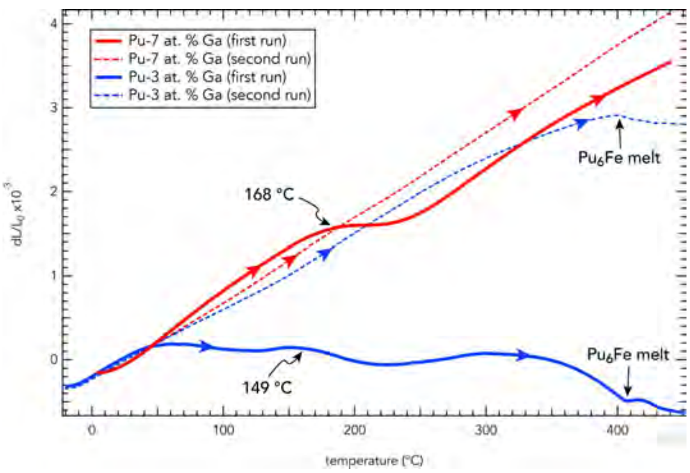
**Peer-reviewed*

Materials for the Future

Aging and Metastability of Delta-Phase Plutonium

Jeremy Mitchell

20210001DR



Dilatometry is used to measure thermal expansion of materials and is an exceptional technique for evaluating the phase stability of plutonium. This plot shows thermal expansion behavior of as-aged plutonium alloyed with 3 atomic % Ga (56 years old) and 7 atomic % Ga (10 years old). Also shown are duplicate experiments run following the initial experiments. Both aged samples show unexpected features between 100 and 200 °C that are consistent with defect movement and recovery. The lack of these features in the second runs indicate that they are related to aging and possibly incipient phase decomposition. The goal of this project is to understand the stability of plutonium through experiments such as these as well other experimental and theoretical approaches.

Project Description

Plutonium (Pu) is a remarkably complex element, and plutonium alloys exhibit similar complexity in their stability and physical properties. The latter is best and most importantly represented by phase relations within the plutonium-gallium system, with gallium being the most common alloying element for stabilizing delta-phase plutonium at room temperature. Despite intense international interest, the plutonium-gallium phase diagram is surprisingly controversial and lacks clear delineation of phase boundaries. This project will produce significant experimental and theoretical results that will greatly impact our fundamental understanding of Pu. Through integration of microstructure, thermophysical properties, and theory, we will produce a refined phase diagram that is both thermodynamically rigorous and aware of the kinetics of phase decomposition. En route to this larger goal, we will establish and employ novel state-of-the art tools that have yet to be used with Pu. These tools, and the results generated from them, will play critical roles in pushing the science of plutonium aging and manufacturing into the future.

Publications

Journal Articles

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Boden, S. B. and S. C. Hernandez. Investigating the Role of Defects in the Alpha-Beta Phase Transformation of Pu using DFT. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27667)

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**Peer-reviewed*

Investigating how Material's Interfaces and Dislocations Affect Strength (iMIDAS)

Abigail Hunter
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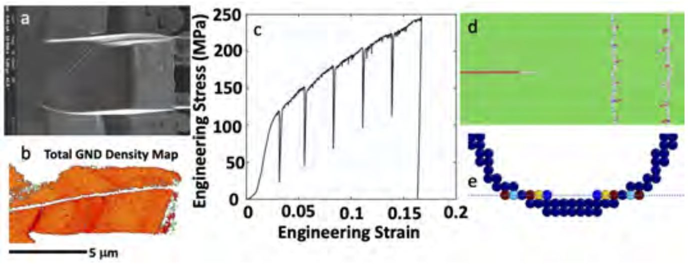

State of the art experiments (Figs. a, b, c) using in situ scanning electron microscopy (SEM) and high resolution electron backscatter diffraction (EBSD) can image lattice rotations and the evolution of geometrically necessary dislocations (Fig. b) correlated with dislocation-grain boundary interactions in bicrystal micro-pillars (Fig a). Similar boundaries can then be modeled using atomistic (Fig. d), meso-scale (Fig. e), and macroscale (not shown) simulation techniques. Together this is an integrated approach that allows the team to investigate the role grain boundary structure and dislocation-grain boundary interactions play in overall mechanical response (Fig. c).

Project Description

The primary mission of Los Alamos National Laboratory (LANL) is stockpile stewardship, and every year LANL must certify that stockpile. In the absence of underground testing, the Laboratory uses modeling and simulation to make this assessment. However, like any mechanical instrument our stockpile is constantly evolving and undergoing changes due to internal and external environmental conditions and decisions by its caretakers. For example, materials age and new manufacturing methods become available. Such changes can lead to microstructural changes within materials and components, thus affecting the expected functionality. Currently, our codes cannot represent this change in properties due to the microstructure. To overcome this shortcoming, we must incorporate more physics into our models regarding the basic mechanisms that drive material yielding and hardening behavior, while keeping the computational cost low. We hypothesize that of known active deformation mechanisms, dislocation grain boundary interactions are one of the dominant mechanisms driving the overall material response. Hence, we plan to incorporate this mechanism into meso and macro-scale models within this project. Success of this project will result in a microstructurally aware macro-scale model available within the codes at LANL.

Publications

Journal Articles

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Dang, K. Q., S. Athikavil Suresh and S. J. Fensin. w21_digbi : Investigating How Material's Interfaces and Dislocations Affect Strength (iMIDAS). . (LA-UR-22-24932)

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**Peer-reviewed*

Topological Quantum Materials for Robust Quantum Computing

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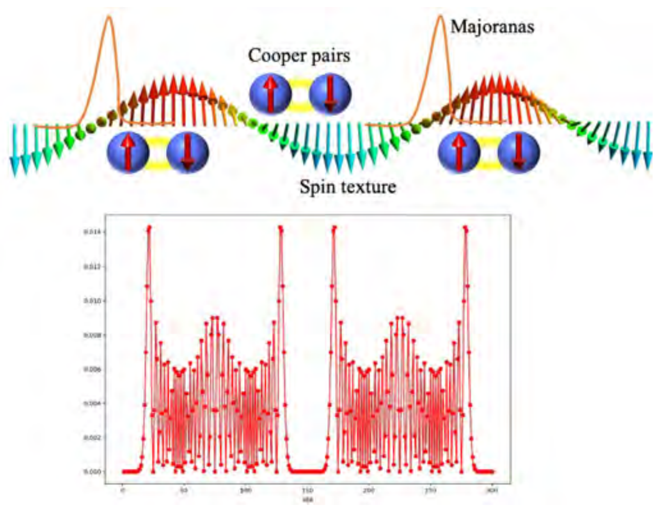

This project contains two main thrusts: topological superconductivity enabled by actinide superconductors and quantum spin liquids enabled by frustrated magnetism. In the figure, we show the Majorana fermion lattice in a topological superconducting state realized in magnetic superconductors. Upper panel: schematic view of emergent Majorana fermion lattice in magnetic superconductors. Lower panel: four Majorana wave functions with overlap in a unit cell obtained by model calculations.

Project Description

A quantum computer performs calculations based on the quantum superposition of different states and holds the promise of solving several classes of problems that are intractable using classical computers. Current quantum computers are built upon quantum two-level systems, such as superconducting qubits; however, the bottleneck preventing quantum computers from solving real-world problems is their short coherence time, i.e., the time scale in which a qubit loses quantum coherence. A fundamentally new paradigm based on novel excitations in topological quantum materials that harnesses the robustness of certain quantum materials can be exploited to achieve fault-tolerant quantum computation. We will develop a materials platform for future quantum computers based on topological quantum materials. We will use the most promising routes to achieve quantum ground states supporting Majorana fermions (MFs), namely topological superconductivity and quantum spin liquid states. Our goals are to establish design principles and provide new materials platforms that host MFs and to develop a combination of probes for unambiguously identifying MFs.

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Rosa, P., S. M. Thomas, C. P. M. Girod, J. D. Thompson and E. D. Bauer. Unusual magnetism and field-induced transitions in Cerium-based materials. Presented at *New directions in strong correlation physics: From strange metals to topological superconductivity*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-28. (LA-UR-22-20362)

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Weiland, A. C., S. S. Fender, F. Ronning, J. D. Thompson, E. D. Bauer, S. M. Thomas and P. Rosa. Correlating Tc and Crystallographic Parameters in UTe2. Presented at *Chirality, Topology, and Unconventional Superconductivity in Sr2RuO4 and UTe2*, Santa Fe, New Mexico, United States, 2021-10-28 - 2021-10-30. (LA-UR-21-30512)

Weiland, A. C., S. S. Fender, M. M. Bordelon, F. Ronning, J. D. Thompson, E. D. Bauer, S. M. Thomas and P. Rosa. The Effects of Annealing in UTe2. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-15 - 2022-03-19. (LA-UR-22-22016)

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Zhu, J. and Y. Huang. Magnetic field-induced chiral spin liquids in transition metal dichalcogenide Moire system. Presented at *Quantum Materials Working Group*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-05. (LA-UR-22-27946)

Posters

Caffer, A., A. Mukkattu Omanakuttan, M. Carvalho, S. Mercena, G. Silva Freitas, H. Pizzi, C. Adriano, E. D. Bauer, J. D. Thompson, F. Ronning, S. M. Thomas, P. Rosa and P. J. Giglio Pagliuso. Tuning the antiferromagnetic ground-state of Ce2RhIn8 by Ga-substitution. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nebraska, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-23001)

M. Girod, C. P., S. M. Thomas, P. Rosa, E. D. Bauer, J. D. Thompson, F. Ronning, J. Zhu, A. Huxley, C. Stevens, R. M. Fernandes and F. Santos. Thermodynamic and electrical transport properties of UTe2 under uniaxial stress. Presented at *29th International Conference on Low Temperature Physics*, Sapporo, Japan, 2022-08-19 - 2022-08-24. (LA-UR-22-28142)

M. Girod, C. P., S. M. Thomas, P. Rosa, F. Ronning, E. D. Bauer, J. D. Thompson, A. Huxley and C. Stevens. Mapping superconductivity with uniaxial stress in UTe2. Presented at *2022 Aspen Winter Conference, New Directions in Strong Correlation Physics: From Strange Metals to Topological Superconductivity*, Aspen, Colorado, United States, 2022-01-24 - 2022-01-28. (LA-UR-22-20243)

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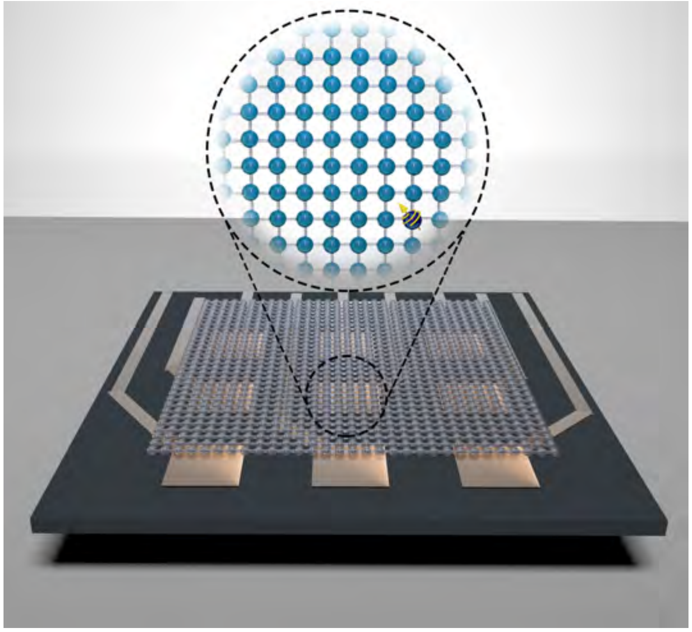
Mukkattu Omanakuttan, A., S. M. Thomas, S. K. Kushwaha, E. D. Bauer, F. Ronning, J. D. Thompson, N. Harrison and P. Rosa. Narrow-gap Kondo insulating ground state of Ce3Bi4Pd3 revealed by applied pressure. Presented at *29th International Conference on Low Temperature Physics (LT29)*, Sapporo, Japan, 2022-08-18 - 2022-08-24. (LA-UR-22-28139)

Weiland, A. C., P. Rosa, S. S. Fender, B. L. Scott, F. Ronning, J. D. Thompson, E. D. Bauer and S. M. Thomas. A Crystallographic Study of UTe2. Presented at *NEW DIRECTIONS IN STRONG CORRELATION PHYSICS: FROM STRANGE METALS TO TOPOLOGICAL SUPERCONDUCTIVITY*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-29. (LA-UR-22-20422)

**Peer-reviewed*

Scalable Molecular Framework Architectures for Qubit Control and State Transduction

Jennifer Hollingsworth
20220047DR



New strategies will be established for ordering, interacting, interfacing and transducing qubits based on molecular spins in metal-organic frameworks. By incorporating the molecules into frameworks, the project team will transform the molecule into a practical material that, as shown here, can be integrated into a solid-state device for individual qubit addressability.

Project Description

Spins-in-molecules are an emerging competitive contender for a "building-block" qubit that can enable real-world quantum technologies from quantum computing to cryptography, communication and sensing. However, molecular spin-qubits are not yet the ubiquitous solution to broad implementation of the quantum advantage. A significant leap in development is needed that entails moving beyond molecular design to molecular assembly and device integration to address qubit scalability, deterministic qubit-qubit interactions and communication with the outside world. In a multidisciplinary effort supported by a strong experiment-theory feedback loop, we will study this problem using metal-organic framework (MOF) chemistry. MOFs provide versatility in organizing building-block molecular units with controlled spacing and the precision afforded by a crystalline material. They are also an ideal synthetic platform for interfacing molecules with solid-state devices, i.e., transforming molecules into solid-state materials. Our work will establish the fundamental science for a materials-by-design approach to qubit-MOF development, along with a series of key results: (1) First intentional entanglement between qubits in a MOF toward quantum-gate operations/quantum-information processing; (2) First voltage controlled initialization/readout of qubits in an array and achieving individual addressability; (3) Creation of a functional hybrid spin-optical state that uniquely enables non-contact initialization/readout of the quantum state in a telecom photon.

Publications

Journal Articles

Li, H., S. A. Shah, A. R. S. Kandada, C. Silva, A. Piryatinski and E. R. Bittner. The Optical Signatures of Stochastic Processes in Many-Body Exciton Scattering. Submitted to *Annual Review of Physical Chemistry*. (LA-UR-22-26542)

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Mozyrsky, D. V., N. Sinitsyn and V. N. Gorshkov. Phase transition in fluctuations of interacting spins at infinite temperature. Submitted to *Physical Review Letters*. (LA-UR-23-23188)

Owczarek, M. T., M. Lee, S. Liu, E. R. Blake, C. S. Taylor, G. A. Newman, J. C. Eckert, J. H. Leal, T. A. Semelsberger, H. Cheng, W. Nie and V. Zapf. Near-Room-Temperature Magnetoelectric Coupling via Spin Crossover in an Iron(II) Complex. 2022. *Angewandte Chemie International Edition*. e202214335. (LA-UR-22-31219 DOI: 10.1002/anie.202214335)

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Reports

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Presentation Slides

Bowes, E. G., J. A. Hollingsworth and N. A. Malone. Synthesis of PbS/CdS/Cu2xS Core/Shell/Shell Quantum Dots. . (LA-UR-22-30201)

Dolgopolova, E. Advancing Manufacturing Science in the Context of Nano- and Quantum Technology. . (LA-UR-22-25513)

Dolgopolova, E. Controlled growth of MOF nanocrystals. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28695)

Greer, S. M. Electron paramagnetic resonance studies of f-element complexes. Presented at *From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25504)

Hollingsworth, J. A. Nanocrystal Quantum Emitters: From the Flask to Photonic (Quantum) Devices). Presented at *The International Conference of Quantum, Nonlinear & Nanophotonics ICQNN'2022*, Jena, Germany, 2022-09-05 - 2022-09-09. (LA-UR-22-31148)

Hollingsworth, J. A. Designing optical nanomaterials to be the ideal partners for solid-state spin qubits. Presented at *TSRC Workshop: From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25238)

Hollingsworth, J. A. Nanocrystal Quantum Emitters: From the Flask to Photonic (Quantum) Devices. Presented at *Northern Arizona University Seminar, Applied Physics and Materials Science and the Center for Materials Interfaces in Research and Applications*, Flagstaff, Arizona, United States, 2022-09-22 - 2022-09-22. (LA-UR-22-31147)

Hollingsworth, J. A., E. Dolgopolova and G. G. Sands. The Synthesis of a Covalent Organic Framework Toward a Scalable Array of Qubits. . (LA-UR-22-32041)

Jones, A. C. Deterministic creation, characterization, and manipulation of nanostucture-based quantum emitters using scanning probe microscopy techniques. Presented at *From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25445)

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E. McClure, C. E. ODMR set-up and theory of nitrogen-vacancy centers in diamond. . (LA-UR-22-29794)

Mishra, S., E. G. Bowes, C. T. Trinh, J. A. Hollingsworth, H. Htoon and A. C. Jones. Inducing Chirality in Single Photon Quantum Emitter Photoluminescence via the Chiral Induced Spin Selectivity Effect. Presented at *APS March Meeting*, Los Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22351)

Owczarek, M. T., M. Lee, W. Nie and V. Zapf. Close-to-room-temperature magnetoelectric coupling via spin crossover in Fe(II) molecule-based compound. Presented at *From*

Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25338)

Sands, G. G. The synthesis of a covalent-organic framework for applications in quantum computing. . (LA-UR-22-27728)

Zapf, V. Magnetism in quantum information&sensing. . (LA-UR-23-21727)

Zhang, S., F. Bahrami, F. Tafti, M. Lee and V. Zapf. Stabilizing the Kitaev spin liquid state in Ag3LiIr2O6 with high magnetic fields. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21905)

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Zhang, Y. Quantum electronic structure theory and first-principles modeling of spin-phonon relaxation. Presented at *TSRC Workshop ``From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information"*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25417)

Posters

Malatesta, R. A., A. Piryatinski, E. Bittner and C. Silva Acu \xc3\xb1a. Probing quantum correlations in molecular systems with polarization-entangled photons. . (LA-UR-22-27659)

Malatesta, R. A., A. R. S. Kandada, A. Piryatinski and C. A. Silva. Questioning the spin-entanglement of singlet fission intermediates: quantum-light spectroscopy of TIPS-tetracene. Presented at *Gordon Research Conference (GRC) - Electronic Processes in Organic Materials*, Lucca, Italy, 2022-06-26 - 2022-07-01. (LA-UR-22-25780)

Younas, N. Building a Quantum computer using a molecular spins.. . (LA-UR-22-27636)

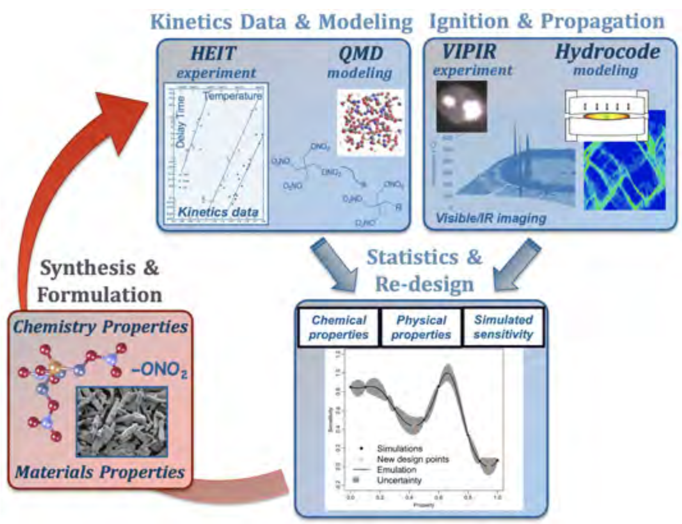
**Peer-reviewed*

Materials for the Future

Directed Research
Continuing Project

Next Generation Probes of Explosive Sensitivity in the Sub-shock Regime

Virginia Manner
20220068DR



In order to understand explosive initiation under low-speed impacts, the project team will apply high throughput experimental tests to measure kinetic properties and visualize ignition and propagation phenomena on explosives synthesized in our labs. These tests will be backed by state-of-the-art theory, simulation, and statistical analysis in an iterative process.

Project Description

The development of new and novel explosives fills a critical need in the Department of Energy (DOE)/National Nuclear Scieance Administration's (NNSA) mission. We can generally identify a powerful, high performance explosive at early stages of development through its high density, heat of formation, and chemical composition. Unfortunately, we lack analogous design guidelines for identifying explosives with good handling safety, which concerns the ease with which violent reactions can be started unintentionally by low-speed impacts, for instance. This means that the development of new explosives is slow, laborious, and expensive due to repeated cycles of scale-up and empirical safety testing. We shall pursue a new approach whereby new experimental tests and theory and simulation capabilities are developed and applied to deconvolute the main factors that contribute to the initiation of reactions in explosives, namely chemical kinetics and the mechanisms responsible for heat generation. By establishing a fundamental mechanistic understanding of explosive sensitivity in the low-speed impact regime, we shall provide reliable and validated guidelines that will inform the design of sensitivity properties into novel explosives for the DOE/NNSA.

Publications

Journal Articles

Cheng, R. M., M. Zecevic, J. D. Moore, M. J. Cawkwell and V. W. Manner. Large Deformation GNARLYX Hydrocode Simulations of the Drop Weight Impact Experiment. Submitted to *AIP Conference Proceedings*. (LA-UR-22-31759)

Davis, J. V., F. W. I. Marrs, A. C. Burch, N. M. Lease, M. J. Cawkwell and V. W. Manner. Prediction of Impact Sensitivity, Heat of Formation and Heat of Explosion using Atomic Connectivity. Submitted to *AIP Conference Proceedings*. (LA-UR-22-31091)

Grennan, H. p., A. C. Burch, B. C. Tappan, V. W. Manner and D. F. Bahr. Addressing nanomechanical testing irregularities in molecular organic crystals to determine mechanical properties. Submitted to *Journal of Materials Research*. (LA-UR-23-22752)

Lease, N. M., K. D. Spielvogel, J. V. Davis, J. T. Tisdale, L. M. Klamborowski, M. J. Cawkwell and V. W. Manner. Halogenated PETN Derivatives: Interplay Between Physical and Chemical Factors in Explosive Sensitivity. Submitted to *Chemical Science*. (LA-UR-23-21991)

Lease, N. M., K. D. Spielvogel, J. V. Davis, J. T. Tisdale, L. M. Klamborowski, M. J. Cawkwell and V. W. Manner. Supplemental Information Halogenated PETN Derivatives: Interplay Between Physical and Chemical Factors in Explosive Sensitivity. Submitted to *Chemical Science*. (LA-UR-23-22896)

Moore, J. D., R. M. Cheng, M. Zecevic, M. D. Holmes, M. J. Cawkwell and V. W. Manner. VIPIR: A High-Throughput Drop-Weight Impact Instrument for Imaging the Initiation and Propagation of Reactions in Energetic Materials. Submitted to *AIP Conference Proceedings*. (LA-UR-22-31549)

Skrabacz, D. A., J. A. Heidemann, M. C. Campbell, A. G. J. Morinec, D. G. Tasker, K. D. Spielvogel, M. J. Cawkwell and V. W. Manner. Development and Modeling for A Small-Scale, Rapidly Heated High Explosives Initiation Time (HEIT) Experiment. Submitted to *AIP Conference Proceedings*. (LA-UR-22-31756)

Zecevic, M., M. J. Cawkwell, R. M. Cheng, V. W. Manner and D. J. Luscher. Eulerian finite element simulations of the drop weight impact test with a dislocation density-based continuum model. Submitted to *AIP Conference Proceedings*. (LA-UR-22-31671)

Reports

Cawkwell, M. J., N. M. Lease and V. W. Manner. Comparison of Computational Approaches for Deriving Explosive Kinetics and Sensitivity. Unpublished report. (LA-UR-22-30558)

Presentation Slides

Cawkwell, M. J., J. V. Davis, N. M. Lease, F. W. I. Marrs, A. C. Burch, S. R. Ferreira and V. W. Manner. Model for explosive sensitivity using enthalpy of explosion and effective trigger linkage kinetics. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-25729)

Cawkwell, M. J., M. Zecevic, F. L. Addessio, D. J. Luscher, N. Mohan, R. T. Perriot and K. J. Ramos. Expediting HE manufacture through scale-bridging simulations: Electronic to mesoscale. Presented at *High Explosive Manufacturing Modernization Workshop*, Socorro, New Mexico, United States, 2022-06-28 - 2022-06-30. (LA-UR-22-25770)

Cawkwell, M. J., R. M. Cheng, J. D. Moore, M. Zecevic and V. W. Manner. Understanding ignition in the VIPIR experiment. . (LA-UR-23-21587)

Cheng, R. M., M. Zecevic, J. D. Moore, M. J. Cawkwell and V. W. Manner. Large deformation GnarlyX hydrocode simulations of the drop weight impact experiment. Presented at *22nd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK22)*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26411)

Cheng, R. M., M. Zecevic, M. J. Cawkwell, F. W. I. Marrs and V. W. Manner. Drop weight impact thermomechanics with GnarlyX multi-physics hydrocode simulations. Presented at *American Physical Society March Meeting 2022*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22027)

Lease, N. M., M. D. Holmes, M. A. E. Erickson, L. M. Klamborowski, E. G. Francois and V. W. Manner. Crush Gun Impact Testing: Analysis of Ignition Sites in Sensitive and Non-Sensitive Explosives. Presented at *MACH Conference*, Annapolis, Maryland, United States, 2022-04-06 - 2022-04-08. (LA-UR-22-23021)

Lease, N. M., V. W. Manner, L. M. Klamborowski and G. W. Brown. Tuning Physical and Chemical\xc2\xa0properties of explosives through Synthetic Modifications. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-02-17. (LA-UR-22-22005)

Lease, N. M., V. W. Manner, M. J. Cawkwell, K. D. Spielvogel, L. M. Klamborowski and J. V. Davis. Halogen substitution on PETN framework: An energetic material sensitivity study. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-25719)

Manner, V. W., F. W. I. Marrs, J. V. Davis, M. J. Grosskopf and M. J. Cawkwell. Trends in a large dataset of historical explosive handling sensitivity experiments. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-07. (LA-UR-23-22210)

Manner, V. W., M. J. Cawkwell, F. W. I. Marrs and N. M. Lease. Utilizing Novel Nitrate Ester Explosives to Interpret

Sensitivity Trends. Presented at *Gordon Research Conference (GRC) - Energetic Materials*, Manchester, New Hampshire, United States, 2022-06-26 - 2022-06-26. (LA-UR-22-25353)

Manner, V. W., M. J. Cawkwell, M. Zecevic, J. D. Moore, N. M. Lease and R. M. Cheng. Investigating the importance of chemical and physical properties of explosives in drop weight impact testing. Presented at *MACH Conference*, Towson, Maryland, United States, 2023-04-05 - 2023-04-05. (LA-UR-23-23063)

Manner, V. W., N. M. Lease, M. J. Cawkwell, J. V. Davis and L. M. Klamborowski. Synthetic Functionalization and Reaction Kinetics of Pentaerythritol Tetranitrate (PETN) Derivatives. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-06-17. (LA-UR-22-25555)

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Zecevic, M. Modeling of large scale plastic deformation during VIPIR experiment. . (LA-UR-23-20252)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Modeling the mesoscale dynamics of PBX: Algorithmic challenges, solutions, and applications\xc2\xa0. Presented at *Conventional High Explosives Grand Challenge*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-10. (LA-UR-21-32004)

Zecevic, M., M. J. Cawkwell, R. M. Cheng, V. W. Manner and D. J. Luscher. Eulerian finite element implementation of a dislocation density-based continuum model with application to simulations of drop weight impact test. Presented at *2022 APS Topical Group on Shock Compression of Condensed Matter (SCCM) Biennial Meeting*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-25942)

Zecevic, M., M. J. Cawkwell, R. M. Cheng, V. W. Manner and D. J. Luscher. Eulerian finite element implementation of a dislocation density-based continuum model with application to simulations of drop weight impact test. Presented at *2022 APS Topical Group on Shock Compression of Condensed Matter (SCCM) Biennial Meeting*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26455)

Posters

Davis, J. V., F. W. I. Marrs, A. C. Burch, N. M. Lease, M. J. Cawkwell and V. W. Manner. Prediction of Impact Sensitivity, \xce\x94Hf and Q using Atomic Connectivity. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-21915)

Grennan, H. P., A. C. Burch, V. W. Manner and D. F. Bahr. ADDRESSING IRREGULAR NANOMECHANICAL RESPONSE IN MOLECULAR CRYSTALS. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-24. (LA-UR-23-22516)

I. Marrs, F. W., M. J. Grosskopf, J. V. Davis, M. J. Cawkwell and V. W. Manner. Identifying chemical determinants of impact sensitivity using causal network regression. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-20772)

I. Marrs, F. W., M. J. Grosskopf, J. V. Davis, M. J. Cawkwell and V. W. Manner. Identifying chemical determinants of impact sensitivity using structural equation modeling. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-02-09. (LA-UR-23-21903)

Moore, J. D., M. Zecevic, V. W. Manner, M. J. Cawkwell and M. D. Holmes. Characterization of Energetic Materials During Impact with Reaction Imaging and Modeling. Presented at *MACH Conference*, Virtual, Maryland, United States, 2022-04-06 - 2022-04-08. (LA-UR-22-23034)

Moore, J. D., R. M. Cheng, M. Zecevic, M. D. Holmes, M. J. Cawkwell and V. W. Manner. Designing a High-Throughput Drop-Weight-Impact Instrument for Real-Time Reaction Imaging of Energetic Materials. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-25470)

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**Peer-reviewed*

Proximity Effects at Meso-, Nano-, and Atomic Scales: A New Path to Quantum Functionalities

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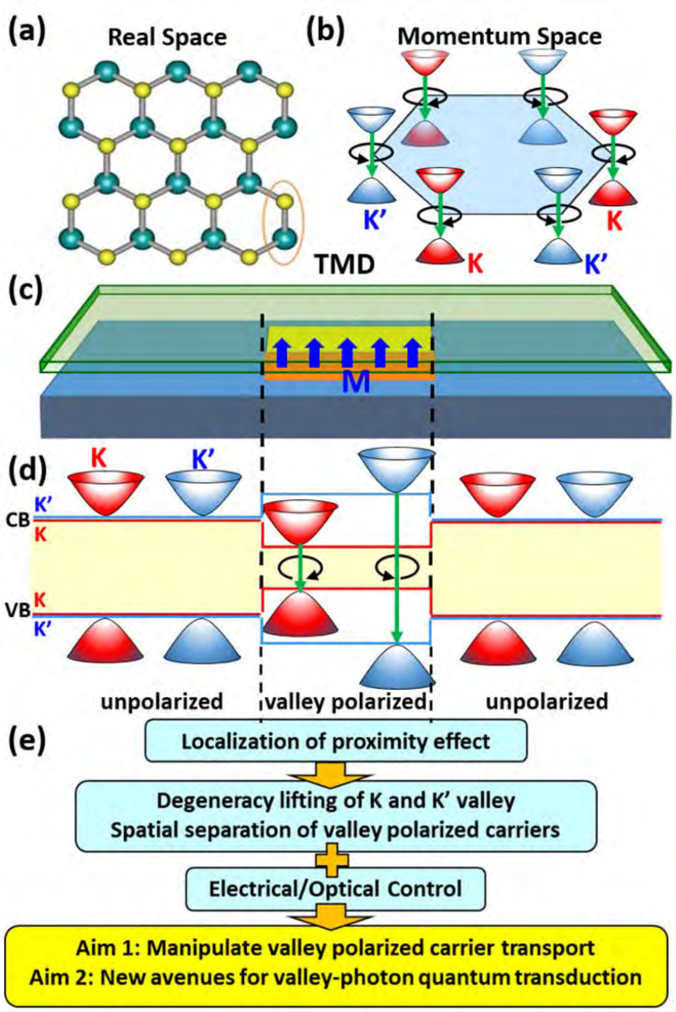

In the image above, atomically thin semiconductors (a) Allow storing and manipulation of information in their valley pseudo spin states (K and K') (b) Full exploitation of this unique property demand lifting energy degeneracy of these two states. The innovation of this project is to couple the semiconductor layer to meso-, nano-, or atomic scale magnets (c) Such that degeneracy of K and K' pseudo spin states were lifted only in the region where two materials are in direct contact. (d) Our research aims to exploit such a localized proximity interaction to realize functionalities in transport and transduction of quantum information (e).

Project Description

Devices based on quantum phenomena are rapidly emerging as enablers for new classes of sensors and detectors as well as for quantum information technologies. Operation of almost all of these devices relies on the ability to generate, manipulate, and detect truly quantum degrees of freedom (DOF), such as spin-up or spin-down state of electrons, or the so-called "valley pseudospin" DOF that is accessible in atomically-thin 2-Dimensional semiconductors. Here, we propose an original approach to significantly broaden the functionality of atomically-thin semiconductors by exploiting novel proximity effects – the phenomenon by which a thin material acquires magnetic properties of an adjacent material via quantum-mechanical interactions. A key innovation of our proposed work is to localize proximity effects to meso-, nano- and atomic scales, rather than inducing effects globally. This will (1) enable an unprecedented ability to manipulate valley pseudospin transport, and (2) open new avenues for transfer of information between valley pseudospin and photon quantum states. With these two aims, we expect our project to bring transformational breakthroughs in the emerging field of "valleytronics", where valley pseudospin is exploited to store and carry information, as well as photonic quantum technologies promising eavesdropping proof communications.

Technical Outcomes

The project resulted in groundbreaking contributions to basic understanding of magnetic proximity effects. New avenues to exploit the effects toward achieving quantum functionalities were revealed. Significant accomplishments: (1) discovery of asymmetric magnetic proximity interaction in molybdenum diselenide ($MoSe_2$)/chromium bromide ($CrBr_3$) heterostructure evidencing that prior understanding of the phenomenon is fundamentally incomplete, and (2) demonstration of the first chiral quantum light generation via nano-scale engineering of proximity interaction in tungsten diselenide (WSe_2)/nickel phosphorus trisulfide ($NiPS_3$) heterostructure.

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**Peer-reviewed*

Control Of Microstructural Instabilities in Composites (COMIC): A Pathway to Realizing Damage Resistant Metals

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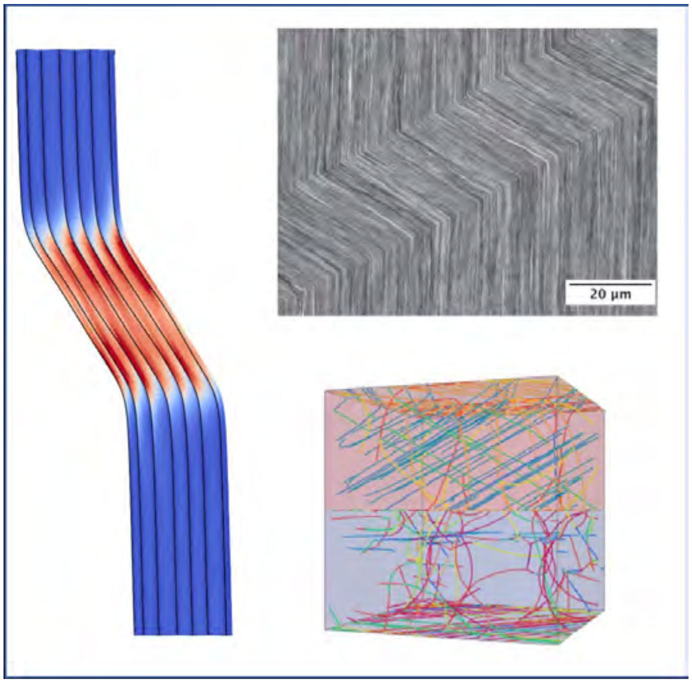

Anticipating the mechanical failure of metals is complex. Los Alamos National Laboratory has developed new models, and designed new materials, to predict how the onset of mechanical instabilities correlates with the fingerprint of the microstructure of metals with tailor made interfaces. These models could be used to design new metals with outstanding mechanical response.

Project Description

This project will deliver an integrated multi-scale modeling framework for the prediction of the relationship between metallic microstructure, loading conditions and ductility. In simpler terms, it will provide the ground-breaking tools needed to predict when failure will occur in metallic materials. This will be enabled by processing and characterizing hitherto not explored/ exploited nanometallic composites such as to allow for the validation of a generalized failure model. As a metric of success, this model will be used to design composites with superior ductility. In the long term, Control Of Microstructural Instabilities in Composites (COMIC) will pave the way towards modeling and designing more resilient metals processed through conventional or advanced manufacturing techniques. This can have Los Alamos-centered impact within potential transition to the National Nuclear Security Administration's advanced manufacturing development program and national missions in energy security by providing pathways to realize light-weighting.

Technical Outcomes

The project identified new processing routes to manufacture new classes of nanometallic laminates (NMLs). The team discovered new NMLs with outstanding mechanical properties/ mass ratio. An advanced micron-scale modeling capability was developed to study the effects of material interfaces on stress concentration. A new modern polycrystal modeling platform was developed and shown to be able to predict failure by shear localization in metals with complex microstructure.

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**Peer-reviewed*

Quantum Photonics with Semiconductor Nanocrystals

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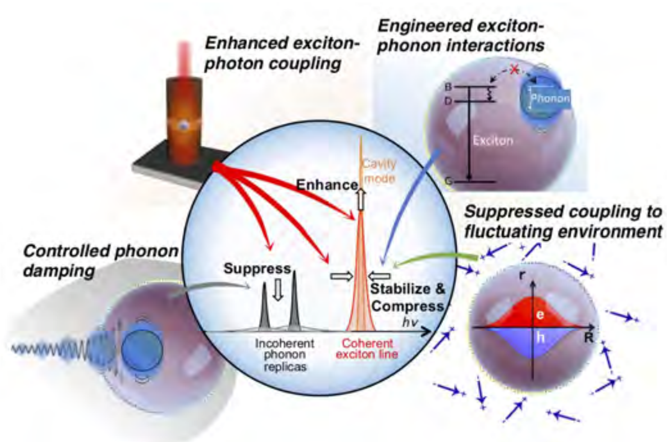

The goal of this project is to exploit unmatched flexibility of colloidal nanocrystals for demonstrating a new class of color-tunable atomic-like sources of quantum light with high-purity single-photon emission and long-lived optical coherence. To accomplish this goal, the project team will manipulate electronic and phonon spectra of the nanocrystals to eliminate spectral instabilities due to fluctuating environment and to suppress dephasing due to electron-phonon scattering. The team will further employ resonant coupling to optical cavities to enhance and sharpen the coherent exciton line and to suppress incoherent phonon replicas.

Project Description

The goal of this project is to exploit the unmatched flexibility of colloidal nanocrystals (NCs) for demonstrating atomic-like single-photon emitters (SPEs) with long-lived optical coherence that is preserved at elevated temperatures. In particular, this project aims to exploit a size-controlled NC band gap for realizing high-fidelity sources of quantum light with an arbitrary wavelength tunable across both visible and NIR spectral ranges. A further objective is to implement integrated NC-photonic circuits using which we will be able to excite a selected NC (or a NC group) and then readout desired information (spectral, temporal, or statistical). This will demonstrate the 'integrability' and scalability of the NC-SPE approach and, in addition, will provide a powerful capability for systematic studies of the effects of controlled photonic environment on SPE-related NC properties. The realization of high-quality NC-based SPEs will lead to a transformational impact in quantum information science (QIS) by addressing the important current challenge of "overcoming the tyranny of low temperature". The availability of highly flexible, colloidal SPEs will facilitate real-life implementations of QIS technologies especially in areas of metrology, sensing, and imaging.

Technical Outcomes

This project has produced multiple advances that contribute to the field of colloidal nanocrystal (NC) single-photon emitters (SPEs), and the general field of generation and manipulation of quantum states of light. These include: (1) the development of approach to enhance coherent "bright-exciton" emission; (2) the demonstration of room-temperature near-infrared SPEs; (3) the realization of electrically pumped optical-gain devices for single-photon amplification; and (4) the demonstration of electrically actuated room-temperature SPEs with record-high emission rates.

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Klimov, V. I. Semiconductor Nanocrystals: Tiny Particles with “Quantum Powers”. . (LA-UR-21-24865)

Marble, C. B. Optical techniques for ion beam physics applications. . (LA-UR-22-27825)

Marble, C. B. and D. Hahm. Dataset of optical properties of CdSe based quantum dots.. Presented at *SPIE Photonics West 2023*, San Francisco, California, United States, 2023-01-28 - 2023-02-02. (LA-UR-22-29604)

Park, Y. Single-Particle Spectroscopy of Colloidal Quantum Dots. Presented at *Sungkyunkwan University Departmental Seminar (Online)*, Online, New Mexico, United States, 2021-05-19 - 2021-05-19. (LA-UR-21-24104)

Park, Y. Laser spectroscopy of colloidal quantum dots. Presented at *Job interview at Korea Advanced Institute of Science and Technology*, Daejun, Korea, South, 2021-05-26 - 2021-05-26. (LA-UR-21-24611)

Robinson, Z. L., H. Jung, Y. Kim, C. Livache, N. Ahn, J. Du, I. Fedin, Y. Park, I. Robel and V. I. Klimov. Bright and fast electrically-excited single-photon emitters from charged quantum dots in a current focusing LED. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-09 - 2022-05-13. (LA-UR-22-24119)

Robinson, Z. L., V. Sayevich, Y. Kim, H. Jung, C. Livache and V. I. Klimov. Vis/NIR CdSe/HgS/CdS Quantum Dots with an atomically-defined emitting interlayer. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-09 - 2022-05-13. (LA-UR-22-24120)

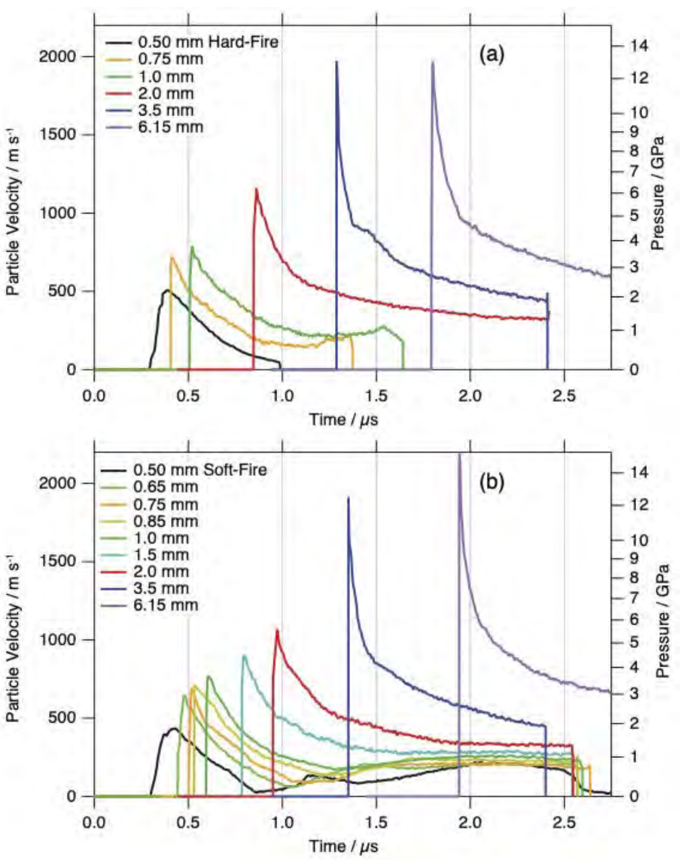
Tretiak, S. and O. Eniodunmo. Electronic Structure of Charged Non-Stoichiometric Quantum Dots. . (LA-UR-22-28206)

Tretiak, S. and S. Gumber. Hot Carrier Relaxation Dynamics in Non-Stoichiometric Quantum Dots. . (LA-UR-22-28205)

**Peer-reviewed*

Understanding How Exploding Bridge-Wire (EBW) Detonators Work

Philip Rae
20210189ER



The build-up to detonation in an exploding bridgewire (EBW) detonator showing unambiguous evidence of the shock-to-detonation process. The colors represent distinct distances from the bursting bridge and the associated time of arrival. The top graph shows the accelerated build-up for a normally fired detonator while the lower shows the slightly delayed buildup for a very weakly fired one. It will be observed that at distances greater than 0.5mm from the bridge a strong and building shock is observed while at 0.5mm a building ramp-wave is observed.

Project Description

There are several detonator technologies of interest to the National Nuclear Security Administration. The oldest, exploding bridgewire (EBW) detonators, are amongst the least understood in terms the fine details of how they actually work. This project aims to dig into the weeds of how they actually function, both to solve the 75 year old scientific mystery and also possibly allow new, better or safer detonators to be designed based on this new knowledge.

Publications

Journal Articles

Feagin, T. A., E. M. Heatwole, P. J. Rae, R. C. Rettinger and G. R. J. Parker. Time-Resolved Nanosecond Optical Pyrometry of the Vapor to Plasma Transitions in Exploding Bridgewires. Submitted to *Scientific Reports*. (LA-UR-21-20261)

Rae, P. J. The modeling of weak shock waves in highly porous powder beds and comments on its relevance to exploding bridgewire (EBW) detonators. Submitted to *Shock Waves*. (LA-UR-20-29268)

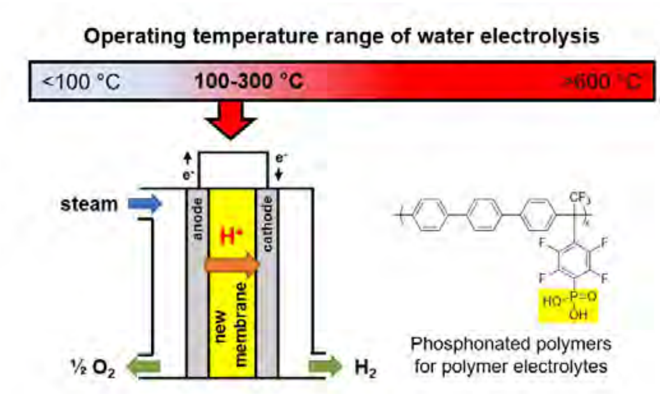
*Rae, P. J. The action-integral and energy to explode short gold wires in ambient air. 2021. *Physics of Plasmas*. **28** (3): 033509. (LA-UR-20-30296 DOI: 10.1063/5.0041067)

*Rae, P. J. and R. C. Rettinger. The effects of electrically exploding gold bridgewires into inert and explosive powder beds. 2021. *Shock Waves*. **31** (8): 887-900. (LA-UR-21-23993 DOI: 10.1007/s00193-021-01041-7)

**Peer-reviewed*

High-Efficiency Steam Electrolysis Using Polymer Electrolyte Membranes

Yu Seung Kim
20210227ER



Novel phosphonated polymer electolytes developed with LDRD support will enable operation of a proton exchange membrane steam-water electrolyzer at 100-300 °C, which will fill the temperature gap between those of current water electrolysis technologies.

Project Description

Hydrogen enables resiliency, energy security, and economic growth across multiple sectors, including renewable and grid electricity. Hydrogen can be produced from diverse domestic feedstocks using a variety of process technologies, including natural gas, coal, nuclear power, and renewable resources. One of the most promising technologies to produce green hydrogen is water electrolysis. Several water electrolysis technologies at the temperature range of 30 to 80 degrees Celsius (C) are under development from early-stage research sponsored by the Department of Energy (DOE), Hydrogen and Fuel Cell Technologies Office. However, those low-temperature electrolysis technologies have low hydrogen production efficiency due to the low operating temperature. In this project, we aim to develop novel conducting materials that enable the operation of water electrolysis at the temperature range of 100 to 200 degrees C. The proposed steam electrolyzer may address the limitations of current water electrolysis technologies by having increased reaction kinetics, higher efficiency and faster hydrogen production rate.

Publications

Journal Articles

Kim, Y. S., E. J. Park, C. C. Arges and H. Xu. Membrane Strategies for Water Electrolysis. 2022. *ACS Energy Letters*. **7** (10): 3447-3457. (LA-UR-22-30093 DOI: 10.1021/acsenergylett.2c01609)

Presentation Slides

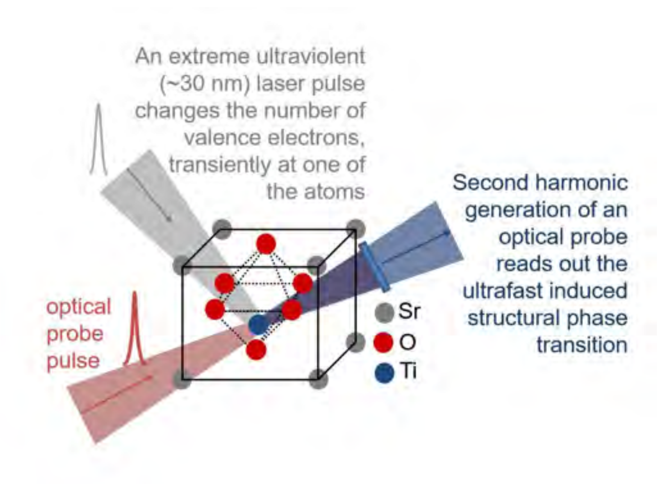
Kim, Y. S. High-temperature polymer electrolytes materials for fuel cells and electrolyzers. Presented at *The 9th International Fuel Cell Workshop 2022*, Kofu, Japan, 2022-11-15 - 2022-11-16. (LA-UR-22-32008)

Kim, Y. S. Research opportunities for high-temperature polymer electrolytes materials. Presented at *Toyota Motors Invite*, | Susono, Japan, 2022-11-17 - 2022-11-17. (LA-UR-22-32009)

**Peer-reviewed*

Ultrafast Control of Material Properties Through Shallow-Core Electrons

Pamela Bowlan
20210290ER



A new strategy for ultrafast control of a material's phase: Extreme Ultraviolet femtosecond laser pulses, ionize, or excite resonant shallow-core excitations in a material, such as the ferroelectrics BaTiO3 or SrTiO3. This laser excitation can induce a structural phase transition, such as switching on or off ferroelectricity or magnetism. A femtosecond optical probe pulse reads out the ultrafast phase of the material using the nonlinear optical effect, second harmonic generation, which is sensitive to the material's symmetry. This type of experiment will be done with our table top light source and also at free electron laser user facilities.

Project Description

As the energy demands of our nation increase, there is a strong need for fundamentally different technology for accessing material properties on demand, for faster more efficient computation and data storage. The idea proposed here, to use femtosecond extreme ultraviolet light pulses for controlling observable material properties such as magnetism and ferroelectricity, offers a novel approach with the potential to be orders of magnitude faster than electronic means of switching. Studying quantum materials with femtosecond extreme ultraviolet light pulses also offers a unique tool for understanding the role of the core electrons and the lattice in leading to a observable properties, which can give to new insight into how to access novel states of matter in the steady state or transiently. The free-electron laser and table top methods that will be developed in this project are also relevant to studying any materials in extreme conditions. Therefore this project has the potential to put Los Alamos National Laboratory at the forefront of quantum materials research and contribute new methods for studying materials in extreme conditions.

Publications

Journal Articles

Peters, w., J. M. Feltman, T. N. Jones, S. Song, M. Chollet, J. Robinson, P. Padmanabhan, L. Foglia, F. Bencivenga, R. Coffe and P. R. Bowlan. Hard X-ray - optical four-wave mixing using a 1 split-and-delay line. Submitted to *Optica*. (LA-UR-22-29673)

Conference Papers

Buckway, T. J. Coherent Tabletop Extreme Ultraviolet Source for Probing and Exciting Ultrafast Magnetization Dynamics. Presented at *Frontiers in Optics + Laser Science*. (Rochester, New York, United States, 2022-10-16 - 2022-10-20). (LA-UR-22-28805)

Reports

Bowlan, P. R. Ultrafast control of material properties through shallow-core electrons. Unpublished report. (LA-UR-22-27583)

Feltman, J. M. Light-matter interaction with X-ray transient Grating. Unpublished report. (LA-UR-22-27826)

Presentation Slides

Bowlan, P. R. Using nonlinear-optics as a fast time-gate for measuring EUV and X-ray FEL pulses. Presented at *WavemiX*, webex, Germany, 2022-06-13 - 2022-06-15. (LA-UR-22-25537)

Bowlan, P. R., P. J. Skrodzki and P. Padmanabhan. Ultrafast control of electrons through shallow-core electrons. . (LA-UR-22-23075)

Feltman, J. M., P. R. Bowlan, T. N. Jones, W. K. Peters, P. Padmanabhan, S. Sanghoon, M. Chollet, J. Robinson, L. Foglia and F. Bencivenga. Light-matter Interaction with X-ray Transient Grating. Presented at *SULI Student Presentations*, Los Alamos, New Mexico, United States, 2022-07-21 - 2022-07-21. (LA-UR-22-27272)

Feltman, J. M., W. K. Peters, T. N. Jones, s. song, M. Chollet, J. Robinson, L. Foglia, F. Bencivenga, R. Coffee, P. Padmanabhan and P. R. Bowlan. Hard-X-ray, optical Transient Grating for probing ultrafast dynamics in solids. Presented at *FIO+LS*, Rochester, New York, United States, 2022-10-17 - 2022-10-20. (LA-UR-22-30860)

Peters, W., T. N. Jones, S. Song, M. Chollet, J. Robinson, L. Foglia, F. Bencivenga, R. Coffee and P. R. Bowlan. X-ray– optical transient grating measurements at LCLS. Presented at *Conference on Light and Electro-Optics (CLEO*, virtual, California, United States, 2021-05-09 - 2021-05-09. (LA-UR-21-24465)

Posters

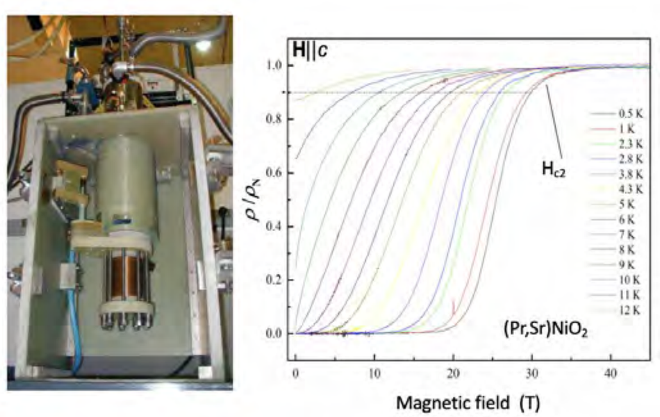
Buckway, T. J. Ultrafast XUV Excitation for Controlling Macroscopic Properties of Materials. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27584)

Buckway, T. J., A. Redd, J. M. Feltman, P. J. Skrodzki, P. Padmanabhan, P. R. Bowlan and R. L. Sandberg. Coherent Tabletop Extreme Ultraviolet Source for Probing and Exciting Ultrafast Magnetization Dynamics. Presented at *Frontiers in Optics and Laser Science conference*, Rochester, New York, United States, 2022-10-17 - 2022-10-20. (LA-UR-22-30440)

**Peer-reviewed*

Unconventional Superconductivity in the Nickelates

Boris Maiorov
20210320ER



The pulsed magnet at Los Alamos provides maximum fields of 65 tesla, more than three times larger than state-of-the-art commercial lab magnets. The high fields, achievable only for short times (~10 ms), is necessary to study high-temperature superconductors. The project team will develop novel fast symmetry resolved techniques to study the newly discovered nickelate superconductors in pulsed magnets. For example, the destruction of superconductivity, signified by zero resistivity, with temperature and field is shown on the right. Such measurements are important for providing a fundamental understanding of emergent phenomena in quantum materials.

Project Description

High-temperature superconductivity is an emergent electronic state of matter that permits perfect conduction of electricity. It is an essential property for future power-grid applications, magnet-technology, and is the foundation for ideas concerning quantum computing. Despite decades of research, it remains one of the greatest unsolved problems in physics. The 2019 discovery of superconductivity in infinite layer nickelate opens a new family of unconventional superconductors for study. This project aims to achieve a fundamental understanding of this new material.

Publications

Journal Articles

Chow, L. E., K. Rubi, K. Y. Yip, M. Pierre, M. Leroux, X. Liu, Z. Luo, S. Zeng, C. Li, M. Goiran, N. Harrison, W. Escoffier, S. K. Goh and A. Ariando. Dimensionality control and rotational symmetry breaking superconductivity in square-planar layered nickelates. Submitted to *Nature*. (LA-UR-23-20556)

Miura, M., G. Tsuchiya, T. Harada, K. Sakuma, H. Kurokawa, N. Sekiya, Y. Kato, R. Yoshida, T. Kato, K. Nakaoka, T. Izumi, F. Nabeshima, A. Maeda, T. Okada, S. Awaji, L. Civale and B. Maiorov. Thermodynamic approach for enhancing superconducting critical current performance. 2022. *NPG Asia Materials*. **14** (1): 85. (LA-UR-22-22302 DOI: 10.1038/s41427-022-00432-1)

Reports

Mizzi, C. A., F. F. Balakirev, B. A. Maiorov and M. Miura. Mid-pulse magnet allows continuous measurements of non-linear voltage characteristics in HTS superconductors. Unpublished report. (LA-UR-23-21097)

Presentation Slides

Maiorov, B. A. New discoveries and opportunities for superconductors in pulsed-high magnetic fields. Presented at *CEC-ICMC 21*, virtual conference, New Mexico, United States, 2021-07-19 - 2021-07-23. (LA-UR-21-26685)

Maiorov, B. A. New discoveries and opportunities for superconductors in high magnetic fields: What can we learn above 40T?. Presented at *Internal Seminar*, Los Alamos, New Mexico, United States, 2021-09-09 - 2021-09-09. (LA-UR-21-28897)

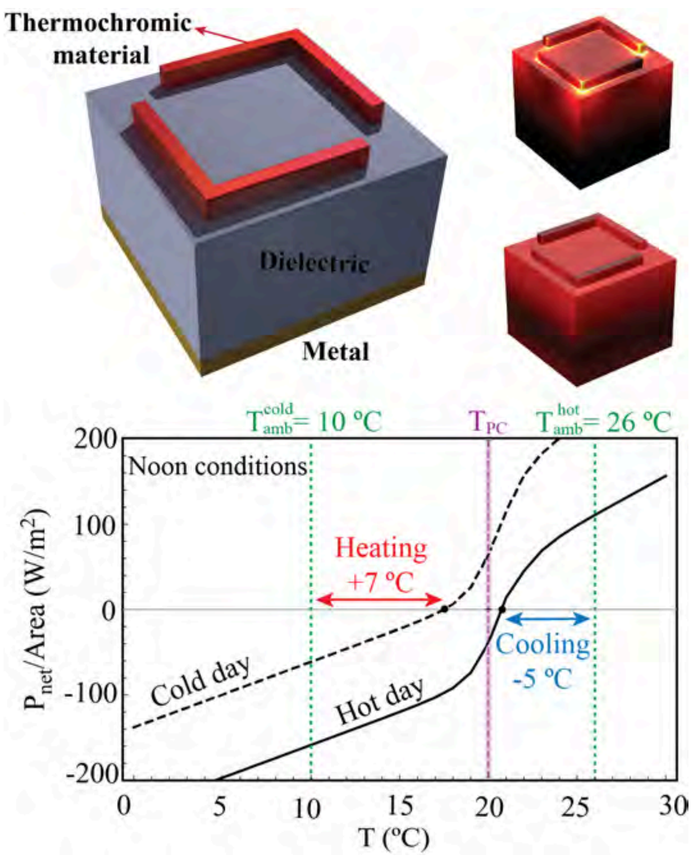
Maiorov, B. A. Challenges and opportunities for Superconductors in High Magnetic Fields. . (LA-UR-21-31299)

Mizzi, C. A., F. F. Balakirev and B. A. Maiorov. Overcoming dH/dt Effects on Non-Linear Electrical Transport in Superconductors. Presented at *NHMFL User Committee Meeting*, Los Alamos, New Mexico, United States, 2022-10-11 - 2022-10-11. (LA-UR-22-30456)

**Peer-reviewed*

Hybrid Thermochromic Nanostructures for Radiative Heat Emergent Functionalities

Wilton Junior de Melo Kort-Kamp
20210327ER



Smart hybrid thermochromic metasurface for passive radiative thermal management near room temperature. The thermochromic nanostructure uses its insulator-to-metal phase-change transition as an autonomous mechanism to self-adjust the device's photonic properties depending on the environment's temperature, allowing for passive radiative cooling and heating.

Project Description

Reducing human reliance on energy-inefficient thermal management systems has taken on renewed urgency to reduce carbon emissions on our warming planet. Particularly, accomplishing environmentally friendly materials for temperature control would strongly impact the United States' energy landscape, where heating and cooling of residential and commercial structures account for about one-third of the electricity use, making them the largest energy expense in the country. The key innovation of this project is to develop phase-change nanostructured materials that passively monitor the ambient temperature and autonomously switch between absorber and emitter states to maintain the temperature close to a desired set point without any energy consumption. Our material platform could solve critical challenges in radiative heat phenomena, including passive radiative cooling technologies, artificial thermal skins for personal temperature regulation, and thermal sensing. Scaled up production of our proof-of-concept metasurfaces could help promote thermochromic photonic systems as a viable energy technology with clear applications to temperature regulation in residential and commercial structures in harsh climates, mitigation of material stresses on structures undergoing thermal cycles, and passive thermal management of micro-satellites. This project will have a positive impact to national energy security as well as strongly impact research in renewable energy, nanotechnology, and nanophotonic sciences.

Publications

Journal Articles

Corey, Z., P. Lu, G. Zhang, Y. Sharma, B. Rutherford, S. Dhole, P. Roy, Y. Wu, H. Wang, A. Chen and Q. Jia. Structural and Optical Properties of High Entropy (La,Lu,Y,Gd,Ce)AlO3 Perovskite Thin Films. 2022. *Advanced Science*. 2202671. (LA-UR-22-30486 DOI: 10.1002/advs.202202671)

Deop-Ruano, J. R., S. Sanders, A. Alabastri, W. J. M. Kort-Kamp, D. A. R. Dalvit and A. Manjavacas. Optical Response of Periodic Arrays of Graphene Nanodisks. 2022. *Physical Review Applied*. **18** (4): 044071. (LA-UR-22-25625 DOI: 10.1103/PhysRevApplied.18.044071)

Sanders, S., L. Zundel, W. J. de Melo Kort-Kamp, D. A. R. Dalvit and A. Manjavacas. Near-Field Radiative Heat Transfer Eigenmodes. Submitted to *PRL*. (LA-UR-21-20930)

*Szilard, D., P. Abrantes, F. Pinheiro, F. Rosa, C. Farina and W. J. de Melo Kort-Kamp. Optical Forces on an Oscillating Dipole Near VO2 Phase Transition. 2021. *Universe*. **7** (6): 159. (LA-UR-21-23943 DOI: 10.3390/universe7060159)

Presentation Slides

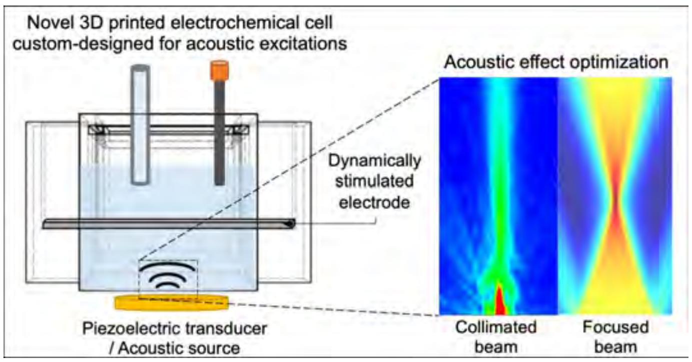
Singh, L., E. B. Qiu, A. E. Cardin, A. Chen, D. A. R. Dalvit, I. K. Schuller, T. S. Luk, A. J. Schuller, W. J. de Melo Kort-Kamp and A. K. Azad. Nanophotonic metasurface for a novel thermal management system. Presented at *American Physical Society (APS) March Meeting*, chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22235)

Singh, L., E. B. Qui, A. E. Cardin, A. Chen, D. A. R. Dalvit, I. K. Schuller, T. S. Luk, A. J. Schuller, W. J. de Melo Kort-Kamp and A. K. Azad. Controlling thermal radiation with a phase-change metasurface. Presented at *Conference on Lasers and Electro-Optics (CLEO) 2022*, San Jose, California, United States, 2022-05-15 - 2022-05-20. (LA-UR-22-24668)

**Peer-reviewed*

Dynamic Catalysis, Advancing Beyond the Sabatier Principle

Siddharth Komini Babu
20210345ER



Current efforts to improve activity of catalytic materials involves a variety of static effects. This work focuses on the integration of dynamic acoustic (mechanical) stimulations on electrocatalyst surfaces to actively promote/control electrochemical processes. For this effort, we have custom-designed a novel 3-dimensional printed electrochemical cell to be able to dynamically apply acoustic vibrations through liquid electrolytes. Fundamental understanding of externally applied dynamic stimuli targets development of next-generation electrocatalysts with controlled functionality applicable to a wide range of electrochemical energy conversion and storage devices. [Image credit: Los Alamos National Laboratory]

Project Description

Our work targets the delivery of scientific discovery and technical breakthroughs in support of Department of Energy and National Nuclear Security Administration missions. Particularly, this project will create a solid foundation for the design of next-generation electrocatalysts with controlled functionality directly applicable to a wide range of Los Alamos National Laboratory programs in electrochemical energy conversion/storage including fuel cells, electrolyzers, batteries, as well as other applications such as chemical synthesis through carbon dioxide (CO2)-electroreduction and electrochemical ammonia synthesis. This project focuses on controlled functionality and predictable performance through the discovery of fundamental material properties with theory-guided innovation at the boundaries of chemistry, physics, and materials science. Our team seeks to create the capability to enable process-to-performance design rooted in fundamental science through advancing our understanding of mechanisms, rates, and performance of materials.

Publications

Reports

Chavez Atayde, L. A., S. Diaz Abad, L. C. Delfin Manriquez, A. J. (. Gupta, E. S. Davis, V. Chillara, E. F. Holby and U. Martinez. Enhanced Oxygen Evolution in Nickel-Based Catalysts via Acoustic Stimulation. Unpublished report. (LA-UR-23-21194)

Chavez Atayde, L. A., S. Diaz Abad, L. C. Delfin Manriquez, A. J. Gupta, E. S. Davis, V. Chillara, E. F. Holby and U. Martinez. Enhanced Oxygen Evolution in Nickel-Based Catalysts via Acoustic Stimulation. Unpublished report. (LA-UR-22-31992)

Chavez Atayde, L. A., S. Diaz Abad, L. C. Delfin Manriquez, V. Chillara, E. S. Davis, S. Maurya and U. Martinez. Enabling Additive Manufacturing of Reactors for Highly Sensitive Electrochemical Systems. Unpublished report. (LA-UR-22-31909)

Presentation Slides

Chavez Atayde, L. A. Electrochemical conversion of pollutants to value-added products using 3D printed parts. . (LA-UR-23-21395)

Chavez Atayde, L. A., V. Chillara, E. S. Davis, E. F. Holby and U. Martinez. Effects of External Acoustic Stimuli Applied to Electrochemical Surfaces and Interfaces. Presented at *Materials Research Society (MRS) Fall Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-08 - 2022-05-08. (LA-UR-22-24293)

Chavez Atayde, L. A. and U. Martinez. Dynamic (Electro)Catalysis: Advancing Beyond the Sabatier Principle. . (LA-UR-21-31952)

Chavez Atayde, L. A. and U. Martinez. Schematic of Experiment. . (LA-UR-22-22752)

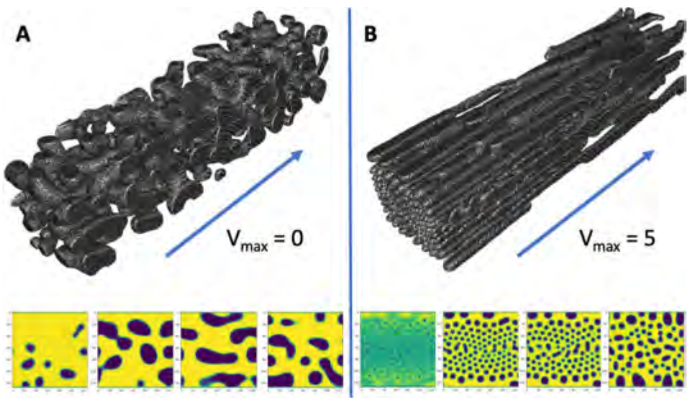
Holby, E. F. w22_electrocat Scientific Highlight. . (LA-UR-23-23064)

Martinez, U., C. M. Benway, L. A. Chavez Atayde, L. C. Delfin Manriquez, T. G. Segni, V. Chillara and E. F. Holby. Effects of Electromagnetic Waves on Electrochemical Systems. Presented at *LANL Summer Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27667)

**Peer-reviewed*

Predicting and Controlling Interfacial Defects in Soft Matter

Cynthia Welch
20210362ER



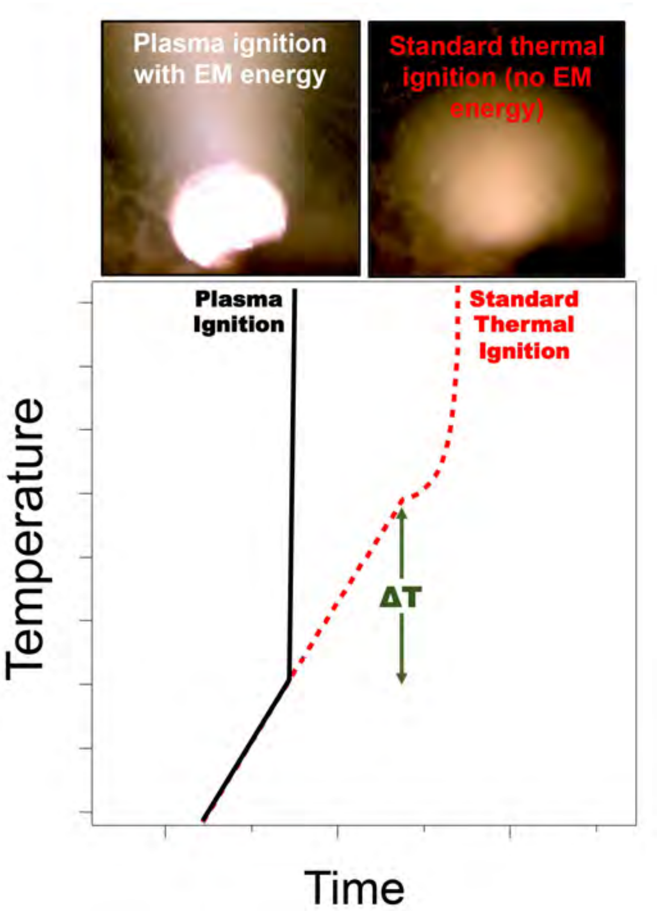
Currently, structural control in additively manufactured polymeric materials is limited to length-scales of multiple microns and above. By 3-dimensional (3D) printing phase-separating block copolymers, the team aims to control morphology at the nano-scale. Images taken from time-dependent Ginzburg-Landau simulations of copolymer phase-separation in a channel demonstrate the effect of flow on morphology development. A simple bicontinuous mesophase results when no flow is present (A), but ordered cylinders form near the channel entry when new material is pumped in (B). Thus, modifying the flow profile could produce novel non-equilibrium structures not otherwise obtainable, giving unique tunable physical properties. (Images produced with ParaView and MatPlotLib.)

Project Description

We will develop both the theoretical understanding needed and the technological tools required to control morphological development during real-world polymer processing. We will apply both time-resolved structural characterization during three-dimensional (3D) printing and a new theoretical method for predicting mesoscale organization. As a result, we will have the ability to fabricate new materials with combinations of properties that are currently unavailable using traditional manufacturing techniques, and we will significantly improve the contribution of additive manufacturing to the new field of polymer upcycling (the process of converting discarded plastics into higher-value materials). In addition, the small footprint and relatively low costs associated with most polymer-based additive manufacturing methods allow for distributed manufacturing; combining this factor with our proposed capability would enable a quick local response to materials needs that arise urgently, e.g., as a result of supply chain interruptions or for production of supplies in remote locations. This project will provide a basis grounded in physics for quickly formulating new feedstocks with imperfect materials.

Manipulating Gas-Phase Chemistry in High Explosive Thermal Decomposition

Amanda Duque
20210399ER



Experimentally, the team shown that the presence of an electromagnetic (EM) field disrupts the thermal decomposition pathway of 1,3,5,7-tetranitro-1,3,5,7- tetraazacyclooctane (HMX), a common stockpile high explosive (HE). A new route of ignition occurs, involving plasma formation, at a temperature lower than what is predicted under typical thermal conditions. Both the plasma ignition and thermal ignition routes begin on the same heating path, but once the EM field is introduced, ignition is initiated. This project is working to quantify and predict the temperature and energy reduction that is achieved for ignition in the presence of an EM field.

Project Description

We recently discovered that our current understanding of thermal ignition of energetic materials may need to be revised -- we observed that the presence of strong electromagnetic (EM) fields significantly alters the fundamental thermal decomposition of a common stockpile high explosive (HE), 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX). This project takes an experimental and modeling approach to uncover the details of this interaction so that we may quantify and predict this behavior for a wide range of energetic materials. We are exploring new and original concepts – compared to traditional thermal effects, almost nothing is known about how EM energy interacts with explosives. For the first time, we will establish a physical-based connection between the materials and explosive properties from the microscale to the bulk continuum response, ultimately to predict and strategically utilize this phenomenon in a broader range of HE systems. The results from this project will not only provide valuable insight into the fundamental decomposition behavior of HE, but also enable a more complete understanding of the shock initiation response of high explosives after and during exposure to EM energy, which is imperative to ensure their safe use in weapon systems during storage, transport and deployment.

Publications

Journal Articles

Lystrom, L. A., A. L. Duque, R. R. S. Burritt and W. L. Perry. Simulating Plasma Ignition of HMX via Microwave Radiation at Substandard Bulk Temperatures. Submitted to *APS GSCCM Conference Proceeding*. (LA-UR-22-31866)

Lystrom, L. A., W. L. Perry and A. L. Duque. A numerical study of electromagnetic enhanced ignition of HMX. Submitted to *Journal of Applied Physics*. (LA-UR-22-26078)

Conference Papers

S. Burritt, R. R., W. L. Perry, A. L. Duque and L. A. Lystrom. Electromagnetic-Induced Thermal Decomposition of RDX. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*. (anaheim,, California, United States, 2022-07-10 - 2022-07-10). (LA-UR-22-31942)

Presentation Slides

S. Burritt, R. R., A. L. Duque, L. A. Lystrom and W. L. Perry. Electromagnetic-Induced Thermal Decomposition of RDX. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, anaheim, New Mexico, United States, 2022-07-11 - 2022-07-11. (LA-UR-22-26069)

Lystrom, L. A. Modeling High Explosives for Safety and Reliability Assurance. . (LA-UR-22-29033)

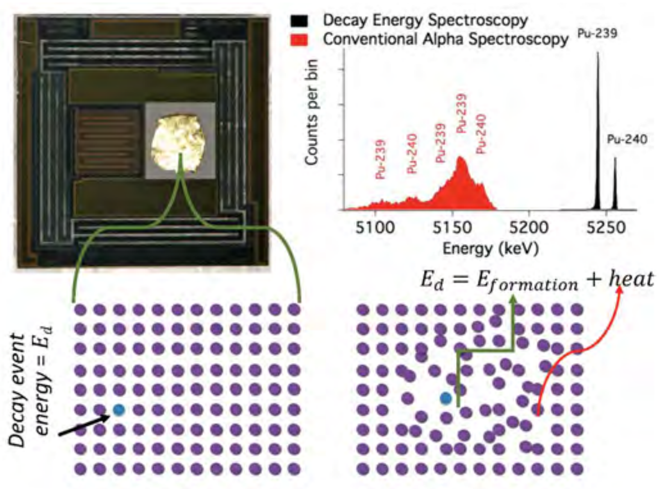
Posters

Lystrom, L. A., A. L. Duque, W. L. Perry and R. R. S. Burritt. Simulating Plasma Ignition of HMX via Microwave Radiation at Substandard Bulk Temperatures. Presented at *22nd SCCM*, anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-26602)

**Peer-reviewed*

Where Does the Energy Go? Refining the Displacements Per Atom Model

Roxanne Tutchton
20220109ER



The ability to analyze material response to structural damage is limited by poor comprehension of the spectrum of point defects created during the damage process. By integrating efforts of cutting-edge calorimetry measurements and advanced ab initio molecular dynamics (AIMD) simulations, the team will refine the displacements per atom (DPA) unit by isolating the effects of damage creation and the resulting defect stored energy from nuclear decay. The development of a quantifiable measurement of damage using the combination of first-principles modeling and ultra-precise calorimetry measurements will be transformational for the study of radiation damage.

Project Description

This fundamental research of Plutonium (Pu) and actinide materials is of paramount importance to national security as an understanding of defects and damage in actinide materials is necessary for an "age aware" model basis and a greater expectation of material performance. We will investigate radiation damage in metallic Uranium (U) and Pu using both experimental techniques and theoretical modeling in order to develop a quantifiable measurement of damage using the combination of first-principles modeling and ultra-precise calorimetry measurements providing a concrete radiation damage source term for studies of self-irradiation damage and aging phenomena. This will be transformational for the study of radiation damage and the field of aging related performance impact for Department of Energy/National Nuclear Security Administration mission relevant materials.

Publications

Presentation Slides

Atta-Fynn, R. Optimal Localized Basis Set for Plutonium. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21760)

Subedi, K. N. and R. M. Tutchton. Self-irradiation damage in \xf0\x9d\x9c\xb6-uranium: An ab initio study. Presented at *APS March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22072)

Tutchton, R. M. Dynamics of Radiation Damage and Defects. Presented at *Postdoc candidate meeting*, Los Alamos, New Mexico, United States, 2021-11-17 - 2021-11-17. (LA-UR-21-31388)

Tutchton, R. M. Planewave Pseudopotential Method: Emphasis on Norm-Conserving Pseudopotentials. . (LA-UR-22-27191)

Tutchton, R. M. Electronic Structure Modeling Strategies for Actinides. Presented at *Meeting at Sandia Nat. Lab*, Albuquerque, New Mexico, United States, 2023-04-11 - 2023-04-11. (LA-UR-23-23492)

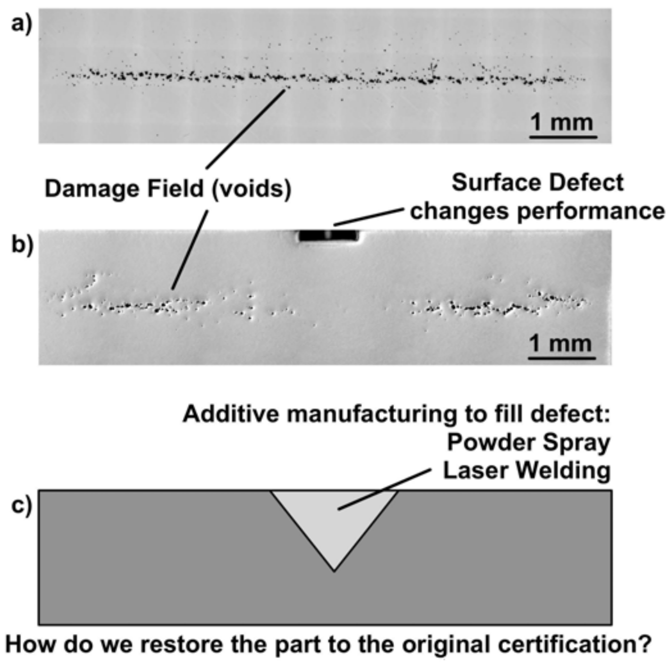
Tutchton, R. M., K. N. Subedi, R. Atta-Fynn and S. C. Hernandez. Modeling Radiation Damage at Atomic Scales. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-02-26. (LA-UR-23-21751)

Tutchton, R. M., W. Chiu, R. C. Albers, G. Kotliar and J. Zhu. Electronic Correlation Induced Expansion of Fermi Pockets in d-Pu. Presented at *Pu Futures*, Avignon, France, 2022-09-25 - 2022-09-30. (LA-UR-22-29722)

**Peer-reviewed*

Additive Manufacturing Repairs for Materials in Extreme Conditions

David Jones
20220152ER



Example of the difference in copper's damage response under shock loading for a) a pristine sample and b) one with a surface defect, a ~1mm wide indent. The defect has clearly changed where and how damage nucleates in the material. This project will investigate the best ways to repair such defects, using additive manufacturing techniques, to bring a part back to its original certified performance. This would avoid costly and time-consuming replacement.

Project Description

Surface defects such as scratches, cracks, or dents, occurring either during manufacturing or from mishandling, can result in costly and time-consuming replacement of mission critical components relevant to National Nuclear Security Administration missions. This work aims to determine whether additive manufacturing techniques, where metal can be added to a part to fill and repair such defects, is suitable for use and certification. By testing a range of different preparation methods and repair processes, we can form a predictive capability for how the repaired material will behave. This will enable this technology to be used to bring components back to their original specification, and potentially mean this production method could be used as a primary advanced manufacturing method for components with tailored behavior.

Publications

Journal Articles

Callanan, J. G., R. Adlakha and M. Nouh. Traveling Wave Thermoacoustic Refrigeration with Real-Time Actively Controlled Boundary Conditions. Submitted to *Journal of the Acoustical Society of America*. (LA-UR-23-22747)

Presentation Slides

Callanan, J. G. Post-grad opportunities at US National Labs. Presented at *University at Buffalo Graduate Student Association Seminar*, Buffalo, New York, United States, 2022-10-14 - 2022-10-14. (LA-UR-22-30761)

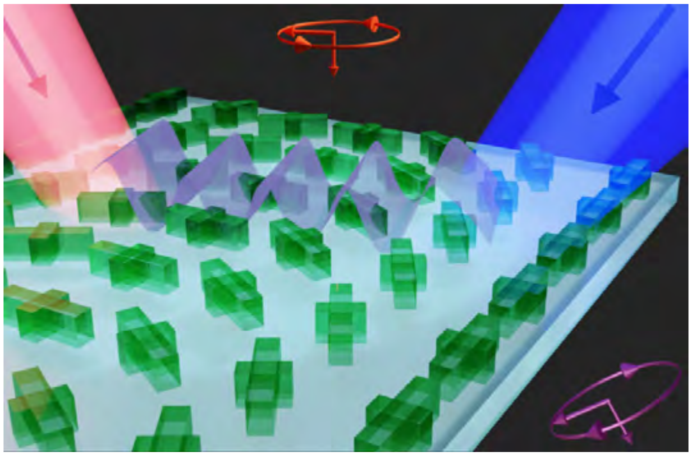
Callanan, J. G., D. R. Jones, S. J. Fensin and D. T. Martinez. Dynamic strength performance of additively repaired small-damage sites in stainless steel. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-23. (LA-UR-23-22599)

Jones, D. R., D. T. Martinez, J. G. Callanan, S. J. Fensin and G. T. I. Gray. Microstructural effects on the shock Hugoniot. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-19. (LA-UR-23-22690)

**Peer-reviewed*

Space-Time Quantum Metasurfaces

Diego Dalvit
20220228ER



Conceptual representation of space-time quantum metasurfaces. An all-optical travelling-wave modulation of the refractive index of a dielectric metasurface induces color-spin-path entanglement on a single photon.

Project Description

Our objective is to develop a whole new concept: space-time quantum metasurfaces (STQMs). Spatio-temporal modulation of the optical properties of quantum metasurfaces will allow to shape the spatial and spectral properties of quantum light on demand, enabling manipulation of quantum photon states in a dynamical photonic platform. We will develop the theory of STQMs and demonstrate the first working prototype for wavefront control of a single photon. STQMs have the potential to bring breakthrough advances in quantum science and technology. This project will help consolidate the Los Alamos National Laboratory trademark with our recently proposed breakthrough concept of space-time quantum metasurfaces, an original Los Alamos work. The project will develop the concept in depth and provide the first experimental demonstration of a working space-time quantum metasurface prototype, enabling the Laboratory to jump to the forefront of photonic quantum technologies. Our work supports Los Alamos National Laboratory/Department of Energy long-term goals on quantum information science and has the potential to impact various programs aimed at harnessing quantum coherence. The developed capabilities will contribute to build future programs on quantum metasurfaces for quantum communications, quantum sensors, and quantum light sources.

Publications

Journal Articles

Deop-Ruano, J. R., S. Sanders, A. Alabastri, W. J. M. Kort-Kamp, D. A. R. Dalvit and A. Manjavacas. Optical Response of Periodic Arrays of Graphene Nanodisks. 2022. *Physical Review Applied*. **18** (4): 044071. (LA-UR-22-25625 DOI: 10.1103/PhysRevApplied.18.044071)

*Muniz, Y., P. P. Abrantes, L. Mart\xc3\xadn-Moreno, F. A. Pinheiro, C. Farina and W. J. M. Kort-Kamp. Entangled two-plasmon generation in carbon nanotubes and graphene-coated wires. 2022. *Physical Review B*. **105** (16): 165412. (LA-UR-21-31553 DOI: 10.1103/PhysRevB.105.165412)

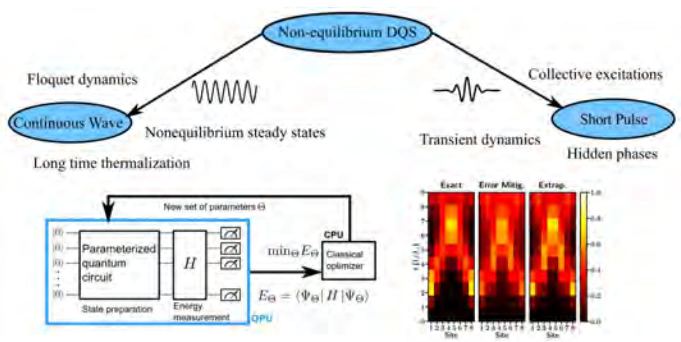
Presentation Slides

R. Dalvit, D. A. Space-Time Quantum Metasurfaces. Presented at *LANL RPI Meeting*, Los Alamos, New Mexico, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-23918)

**Peer-reviewed*

Digital Quantum Simulations for Dynamical Quantum Matter

Jianxin Zhu
20220253ER



Simulations of strongly correlated quantum matter out of equilibrium presents is a significant science challenge. Digital quantum simulations (DQS) is promising to overcome this challenge. With the development of new quantum algorithms such as variational quantum eigensolver (Lower left panel) and efficient time propagation with error mitigation (Lower right panel), the DQS can be applied to study dynamical quantum matter in continuous wave and short pulse excitations regimes for non-equilibrium steady states and transient dynamics. The DQS method for light-matter interactions will help materials design with many possible future applications. [Image credit: Los Alamos National Laboratory]

Project Description

Quantum materials with controlled functionality and behavior will play an important role in next-generation electronic and energy devices. In particular, strongly correlated electron materials (SCEMs) with competing degrees of freedom, provide an unprecedent tunability for emergent states like high-temperature superconductivity and novel magnetism. However, the understanding of SCEMs out of equilibrium, arising from their coupling to a strong external electromagnetic field (e.g., laser pulse), has been a scientific grand challenge. Solely because of strong correlation and coupling, the computational effort to simulate a system of interacting quantum particles scales exponentially in their number, preventing us from describing large-scale quantum systems on classical computers. In this project, we will tackle this challenge by using modern quantum computers to make the first step towards quantum computation of dynamical quantum matter. Specifically, we focus on nonequilibrium dynamics of microscopic models that describe the fundamental physics of quantum materials, extending previous work by including strong light-matter interactions explicitly. Our work will lay an important foundation for the applications of noisy near-term quantum computers to the prediction and characterization of SCEMs. It will enable to significantly speed up the quantum materials design with the aid of future advanced quantum computing hardware.

Publications

**Peer-reviewed*

Journal Articles

Cincio, L., T. Eckstein, R. Mansuroglu, P. Czarnik, J. Zhu, M. Hartmann, Z. Holmes and A. T. Sornborger. Large-scale simulations of Floquet physics on near-term quantum computers. Submitted to *Physical Review X*. (LA-UR-23-22062)

Fauseweh, B. and J. Zhu. Ultrafast Optical Control of Magnetic Order and Fermi Surface Topology at a Quantum Critical Point. Submitted to *Science Advances*. (LA-UR-21-25611)

Khare, A., S. Banerjee and A. B. Saxena. Superposed periodic kink and pulse solutions of coupled nonlinear equations. Submitted to *Journal of Mathematical Physics*. (LA-UR-23-20060)

Khare, A., S. Banerjee and A. B. Saxena. New static solutions of symmetric $\\phi^4$ equation. Submitted to *Annals of Physics*. (LA-UR-23-21202)

*Rehr, J. J., A. P. Kaduwela, R. C. Albers, J. J. Kas and F. D. Vila. Real-space Green's function approach to photoelectron diffraction. 2022. *Journal of Electron Spectroscopy and Related Phenomena*. **259**: 147237. (LA-UR-22-26382 DOI: 10.1016/j.elspec.2022.147237)

Saxena, A. B., F. Cooper, A. Khare, J. F. Dawson and E. G. Charalampidis. Uniform Bose-Einstein Condensates as Kovaton solutions of the Gross-Pitaevskii Equation through a Reverse-Engineered Potential. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-23-21703)

Saxena, A. B., L. Diaz, R. C. Albers and M. Sanati. Dipolar effects on the work function of an alkali-iodide overlayer (XI, X = Li, Na, K, Rb, and Cs) on tungsten surfaces. Submitted to *Physical Review Materials*. (LA-UR-22-29340)

Saxena, A. B. and S. Gupta. Tunable Electrocaloric Effect in Selective Ferroelectric Bilayers via Electrostatics for Microelectronics Thermal Management. Submitted to *Physical Review Applied*. (LA-UR-23-20907)

Zhu, J. and B. Fauseweh. Quantum computing Floquet band structures. Submitted to *Quantum*. (LA-UR-21-31933)

Presentation Slides

Saxena, A. B. Flexocaloric Effects in Ferroic Materials. Presented at *ICOMAT 2022*, Seoul, Korea, South, 2022-03-13 - 2022-03-13. (LA-UR-22-21383)

Saxena, A. B., A. S. Bhalla and R. Guo. A Lesson in the History of Ferroelectricity. Presented at *ICAPMA-JMAG-2021 (virtual)*, Pattaya, Thailand, 2021-12-01 - 2021-12-01. (LA-UR-21-31610)

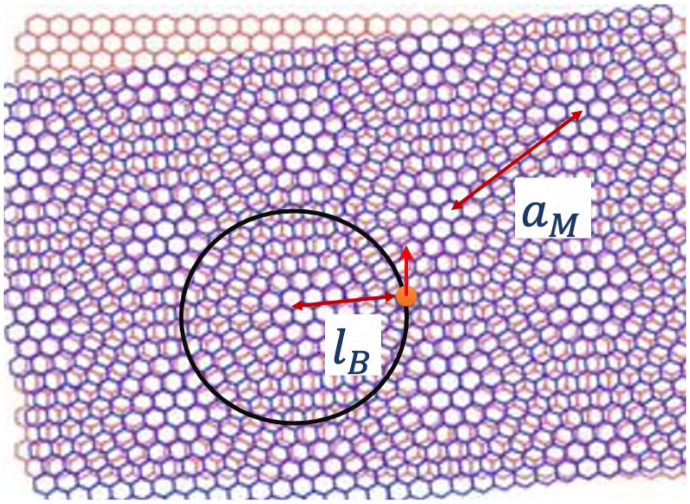
Zhu, J. and B. Fauseweh. Digital quantum simulation of non-equilibrium quantum many-body systems. . (LA-UR-22-24559)

Materials for the Future

Exploratory Research
Continuing Project

Moiré Physics in Quantum Flatland

Shizeng Lin
20220271ER



Schematic view of Moiré superlattice with a lattice period a_M. The black circle denotes an electron cyclotron orbit in a magnetic field, and its radius is defined as the magnetic length l_B.

Project Description

"Moiré Superlattices", which are realized when two atomically-thin crystals are stacked one atop the other, can host many novel quantum states because of the increased length scale. In the presence of a strong magnetic field, the Moire superlattices represent an entire new platform where magnetic field can stabilize an entirely new quantum states of matter that are not possible in atomic crystals. We will investigate the novel quantum states in Moiré Superlattices under a strong magnetic field. These emergent phases either break underlying symmetries and/or possess nontrivial topological order because of strong electronic correlations, with possible application in novel quantum devices and robust quantum computation.

Publications

Journal Articles

Choi, J., C. A. Lane, J. Zhu and S. A. Crooker. Asymmetric magnetic proximity interactions in MoSe2/CrBr3 van der Waals heterostructures. 2022. *Nature Materials*. (LA-UR-22-25241 DOI: 10.1038/s41563-022-01424-w)

Du, K., X. Xu, C. Won, K. Wang, S. A. Crooker and S. W. Cheong. Topological Surface Magnetism and Neel Vector Control in a Magnetoelectric Antiferromagnet. Submitted to *Nature Physics*. (LA-UR-22-24676)

Huang, C. L., N. Wei, I. Blinov, W. Qin, A. MacDonald and T. Wolf. Spin and Orbital Metallic Magnetism in Rhombohedral Trilayer Graphene. Submitted to *Physical Review Letters*. (LA-UR-22-22867)

Huang, C. L., N. Wei, T. Wolf, W. Qin, I. Blinov and A. MacDonald. Functional Renormalization Group Study of Superconductivity in Rhombohedral Trilayer Graphene. Submitted to *Physical Review Letters*. (LA-UR-22-22744)

Li, Z., Q. Yin, Y. Jiang, H. Weng, Z. Zhu, Y. Gao, S. Wang, T. Zhao, J. Cai, H. Lei, S. Lin, Y. Zhang and B. Shen. Visualization of topological magnetic textures near room temperature in quantum magnet TbMn6Sn6. Submitted to *Nature Materials*. (LA-UR-22-30730)

Lin, S. Skyrmion lattice in centrosymmetric magnets with local Dzyaloshinsky-Moriya interaction. Submitted to *Scipost Physics*. (LA-UR-21-32483)

Lin, S. Kondo enabled transmutation between spinons and superconducting vortices: origin of magnetic memory in 4Hb-TaS2. Submitted to *Physical Review Letters*. (LA-UR-22-30653)

Lin, S., S. Sarkar, K. Sun and X. Wan. Topological exact flat bands in two dimensional materials under periodic strain. Submitted to *Physical Review Letters*. (LA-UR-22-32239)

Lin, S., X. Wan, S. Sarkar and K. Sun. Nearly flat Chern band in periodically strained monolayer and bilayer graphene. Submitted to *Physical Review B*. (LA-UR-23-21523)

*Ren, L., L. Lombez, C. Robert, D. Beret, D. Lagarde, B. Urbaszek, P. Renucci, T. Taniguchi, K. Watanabe, S. A. Crooker and X. Marie. Optical Detection of Long Electron Spin Transport Lengths in a Monolayer Semiconductor. 2022. *Physical Review Letters*. **129** (2): 027402. (LA-UR-22-21878 DOI: 10.1103/PhysRevLett.129.027402)

*Tuan, D. V., S. Shi, X. Xu, S. A. Crooker and H. Dery. Six-Body and Eight-Body Exciton States in Monolayer WSe2. 2022. *Physical Review Letters*. **129** (7): 076801. (LA-UR-22-21272 DOI: 10.1103/PhysRevLett.129.076801)

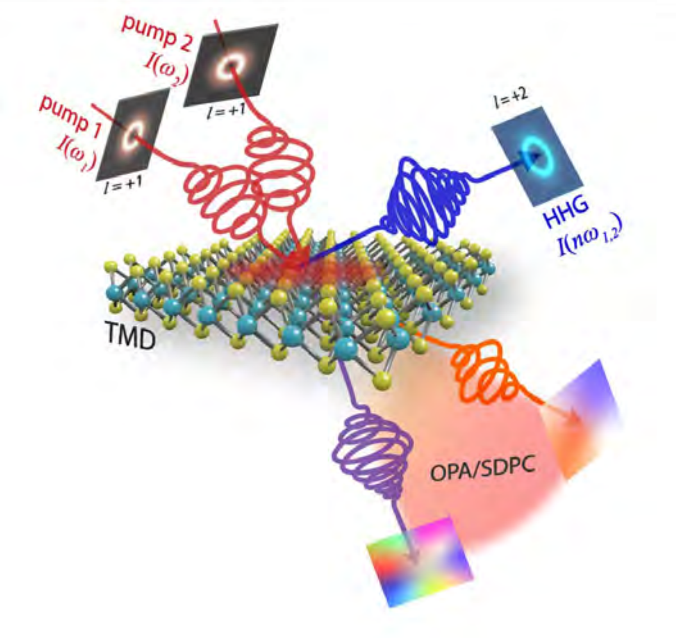
Presentation Slides

Su, Y. Topological moir\xc3\xa9 minibands and correlated Chern insulator from periodically confined massive Dirac fermions. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22321)

**Peer-reviewed*

Nanoscale Nonlinear Optics with a Twist

Prashant Padmanabhan
20220273ER



Orbital angular momentum (OAM) beams can interact with atomically thin transition metal dichalcogenides (TMDs) through nonlinear optical processes including high harmonic generation (HHG), optical parametric amplification (OPA), and spontaneous parametric downconversion (SPDC). These processes make it possible to generate OAM beams with controllable wavelength, quantization, and entanglement for a number of mission-relevant applications, most notably quantum information science.

Project Description

Light can rotate as it travels through space, carrying both spin angular momentum and orbital angular momentum (OAM) (for beams with helical or "twisted" phase fronts, i.e., vortex beams). Unlike spin angular momentum, OAM has an infinite number of quantized integer values. This makes it particularly attractive for applications ranging from optical tweezers to quantum information science (QIS). These applications depend on producing vortex beams with controllable wavelength, quantization, and entanglement, which can be done via nonlinear optics. Previous studies have done this at the macroscale, but future applications will depend on nanoscale implementation. We will address this using atomically thin semiconducting transition metal dichalcogenides for nanoscale nonlinear optics with vortex beams, enabling us to generate widely tunable OAM modes and entangled OAM photons for QIS.
Our proposal directly addresses the Materials for the Future pillar via the development of Materials and Phenomena underpinning Quantum Information Science. It also addresses Basic Energy Science reports on Next Generation Quantum Systems, Quantum Materials, and Ultrafast Science. We thus expect to deliver a robust capability for generating vortex beams with controlled properties at the nanoscale, impacting both fundamental and mission-relevant applications across Los Alamos National Laboratory.

Publications

Presentation Slides

Martinez Milian, L. M., Y. Liu, C. Petrovic, M. T. Pettes, R. P. Prasankumar, S. R. Singamaneni and P. Padmanabhan. Coherent Spin-Phonon Coupling in the Layered Ferrimagnetic Crystal Mn3Si2Te6. Presented at *American Physical Society (APS) March Meeting*, Online, District Of Columbia, United States, 2023-03-20 - 2023-03-22. (LA-UR-23-22773)

Padmanabhan, P. Ultrafast Dynamics in Novel Materials: Uncovering Magnetism, Symmetry, and Topology. Presented at *RPI/LANL Nucleation Workshop on Quantum Materials and Devices*, Los Alamos, New Mexico, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-24041)

Padmanabhan, P. Exploring\xc2\xa0Magnetic Dynamics and Collective Phenomena in Quantum Materials. Presented at *Optical Science and Engineering Seminar at University of New Mexico*, Albuquerque, New Mexico, United States, 2022-12-01 - 2022-12-01. (LA-UR-22-32483)

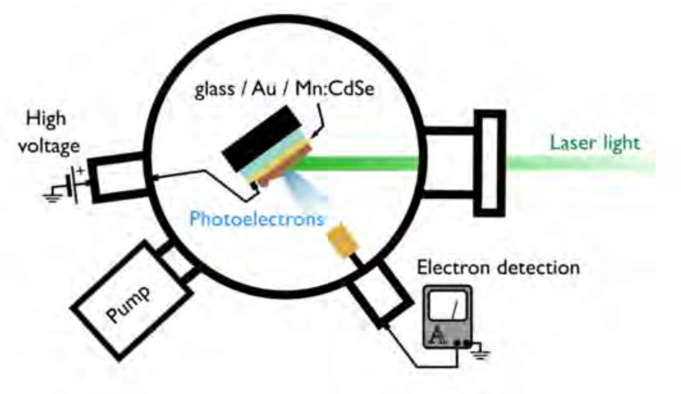
Posters

Yoo, J., Y. Kim, X. Wang, J. D. Watt, B. K. Derby, X. Ma, T. Ahmed, S. Kim, K. Kang, T. S. Luk, Y. J. Hong and A. Chen. Quantum materials research platform prepared by remote epitaxy. Presented at *Two dimensional electronics beyond graphene*, Manchester, New Hampshire, United States, 2022-06-12 - 2022-06-12. (LA-UR-22-25318)

**Peer-reviewed*

High-Efficiency Photoemission Due to Multistep Spin-Exchange Auger Ionization

Victor Klimov
20220279ER



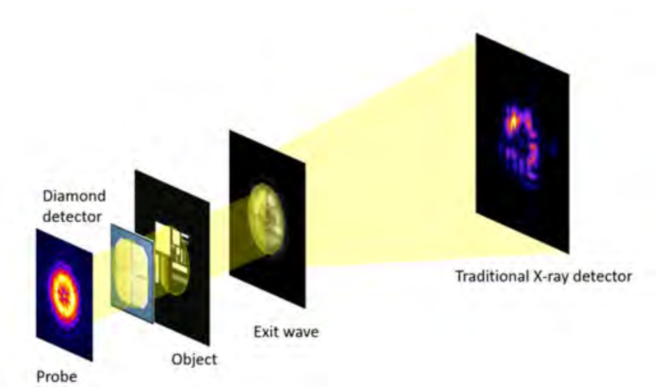
This project will enable a new type of inexpensive, highly robust photocathodes for applications ranging from photomultipliers and night-vision tubes to electron microscopes and free-electron lasers.

Project Description

Photocathodes are essential components of numerous devices from photomultipliers and night-vision tubes to electron microscopes and free-electron lasers. Their operation is based on the effect of 'photoemission' wherein a material emits electrons upon exposure to high-energy, typically, ultraviolet photons. The objective of this project is to explore an alternative process – ultrafast spin-exchange Auger ionization – for achieving highly efficient photoemission driven by visible and, potentially, infrared light. This effect emerges as a result of confinement-enhanced spin-exchange interactions in magnetically-doped colloidal quantum dots. It can enable a new type of inexpensive photocathodes that will combine high photoelectron yields with exceptional robustness stemming from the short-range character of spin-exchange interactions, which makes them insensitive to the external environment.

Diamonds Are Ptychography's Best Friend

Nina Weisse-Bernstein
20220287ER



Ptychography is a powerful lensless imaging techniques that enables near diffraction limited resolution. However, the algorithm is an iterative reconstruction algorithm that can take many iterations. Using transmissive diamond detectors to measure the beam (probe) profile and position can reduce the required iterations by an order of magnitude. Shown in this figure is the illumination of the transmissive diamond detector and object by the x-ray beam (probe). The exit wave from the object is shown, as is the raw data collected by the traditional x-ray detector. This raw data is an input to the ptychography algorithm.

Project Description

This project will create transmissive diamond detectors that will enable beam profile and position measurements at extremely bright x-ray light sources such as x-ray free electron lasers (XFELs). In addition to providing devices that would be useful diagnostics for XFELs such as Linac Coherent Light Source (LCLS) and an eventual Dynamic Mesoscale Material Science Capability (DMMSC) / Matter-Radiation Interactions in Extremes (MaRIE), these devices would enhance the ptychography process by reducing the required iterations per reconstruction. Ptychography is a powerful lensless imaging technique that overcomes the resolution limits associated with traditional x-ray optics. Ptychography is becoming ubiquitous at light sources due to the ability to image with exquisite resolution; this translates to the potential for this work to have impact across a broad range of National Security applications by illuminating structural information across a range of mission relevant materials.

Publications

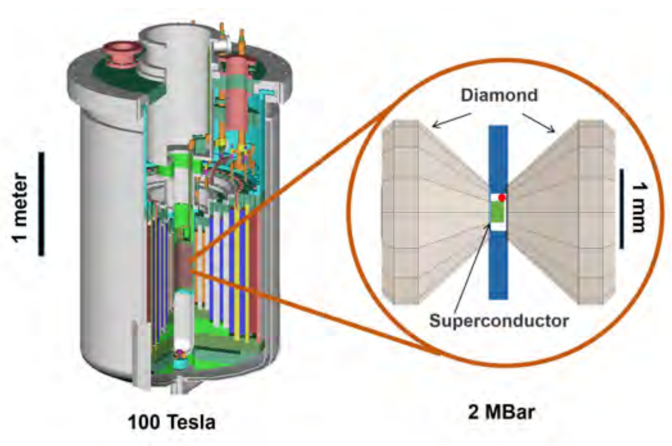
Presentation Slides

Sikes, C. A. Ptychography: Scheduling & Pipelining. . (LA-UR-22-27574)

**Peer-reviewed*

Synthesis and Characterization of Room Temperature Superconductors under Extreme Conditions

Fedor Balakirev
20220299ER



Room temperature hydrogen-rich superconductors form at extreme pressure of several million atmospheres, comparable to pressure at the Earth's core, making their characterization a severe technical challenge. LANL scientists carry out a comprehensive characterization of their structural and electronic properties inside ultrahigh-pressure diamond anvil cells using a combination of synchrotron-based X-ray diffraction and extreme pulsed magnetic fields of 100 Tesla.

Project Description

The proposed work will place Los Alamos National Laboratory in a position of leadership in the rapidly advancing frontier of hydride superconductivity an emerging and prominent area of contemporary material science, where the realization of practical room temperature superconductors becomes more likely with each new discovery. The world will become a different place if superconductivity can replace conventional conductivity in metals, in which friction and heating results in a waste of energy. Room-temperature superconductivity would revolutionize the fields of coherent quantum information, quantum computation, energy security, and transportation, among many others. The project is closely aligned with the Department of Energy/National Nuclear Security Administration Mission Need for Materials to Reduce Energy Consumption since practical superconductor technology will eliminate resistive energy dissipation in electrical wires and circuits. The proposed study also spans several Materials for the Future Science Themes, including the ability to predict response and control of material properties under thermomechanical extremes, the ability to exploit extreme environments to tune materials functionality, and ability to apply electromagnetic extremes at very highest research magnetic fields to characterize the superconducting order in high temperature superconductors (high Tc) materials. The project will couple thermomechanical extremes in a Diamond Anvil Cell(DAC) with the extreme pulsed magnetic fields and high energy domestic and international light sources.

Publications

Journal Articles

*Eremets, M. I., V. S. Minkov, A. P. Drozdov, P. P. Kong, V. Ksenofontov, S. I. Shylin, S. L. Bud'ko, R. Prozorov, F. F. Balakirev, D. Sun, S. Mozaffari and L. Balicas. High-Temperature Superconductivity in Hydrides: Experimental Evidence and Details. 2022. *Journal of Superconductivity and Novel Magnetism*. **35** (4): 965-977. (LA-UR-22-20373 DOI: 10.1007/s10948-022-06148-1)

*Minkov, V. S., S. L. Bud'ko, F. F. Balakirev, V. B. Prakapenka, S. Chariton, R. J. Husband, H. P. Liermann and M. I. Eremets. Magnetic field screening in hydrogen-rich high-temperature superconductors. 2022. *Nature Communications*. **13** (1): 3194. (LA-UR-22-30942 DOI: 10.1038/s41467-022-30782-x)

Reports

sun, d., S. Mozaffari, L. Balicas, F. F. Balakirev, V. S. Minkov, M. E. Eremets, S. Chariton, V. B. Prakapenka, Y. Sun and Y. Ma. Effects of Structural Instability on Superconductivity in Superhydride. Unpublished report. (LA-UR-22-21877)

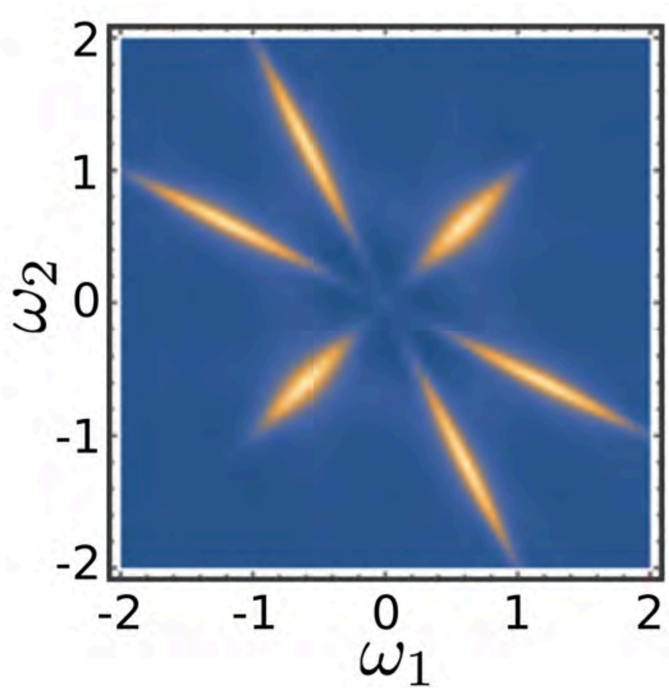
Presentation Slides

Balakirev, F. F. High Field Probe of Superconducting Order in High-Tc Hydrides. Presented at *Maglab user committee meeting*, Los Alamos, New Mexico, United States, 2022-10-11 - 2022-10-13. (LA-UR-22-31019)

**Peer-reviewed*

Fingerprints of Intrinsically Quantum Behavior in Weak Measurements of Macroscopic Systems

Nikolai Sinitsyn
20220325ER



The theoretical prediction for the 3rd order spin correlator of semiconductor quantum dot qubits. It is the guiding prediction for our first experiment.

Project Description

High level goal is to design a measurement technique that will employ purely quantum properties of electrons. This will create a minimally invasive approach to study materials characteristics, including at extremal conditions.

Publications

Journal Articles

Du, K., X. Xu, C. Won, K. Wang, S. A. Crooker and S. W. Cheong. Topological Surface Magnetism and Neel Vector Control in a Magnetoelectric Antiferromagnet. Submitted to *Nature Physics*. (LA-UR-22-24676)

Yan, B. and N. Sinitsyn. An adiabatic oracle for Grover's algorithm. Submitted to *Physical Review Letters*. (LA-UR-22-26707)

Yan, B. and N. Sinitsyn. Randomized Channel-State Duality. Submitted to *Nature Physics*. (LA-UR-22-30432)

Yan, B. and W. H. Zurek. Decoherence factor as a convolution: an interplay between a Gaussian and an exponential coherence loss. 2022. *New Journal of Physics*. **24** (11): 113029. (LA-UR-21-28440 DOI: 10.1088/1367-2630/ac9fe8)

Reports

Touil, A., F. Anza, S. Deffner and J. P. Crutchfield. Branching States as the Emergent Structure of a Quantum Universe. Unpublished report. (LA-UR-22-27917)

Presentation Slides

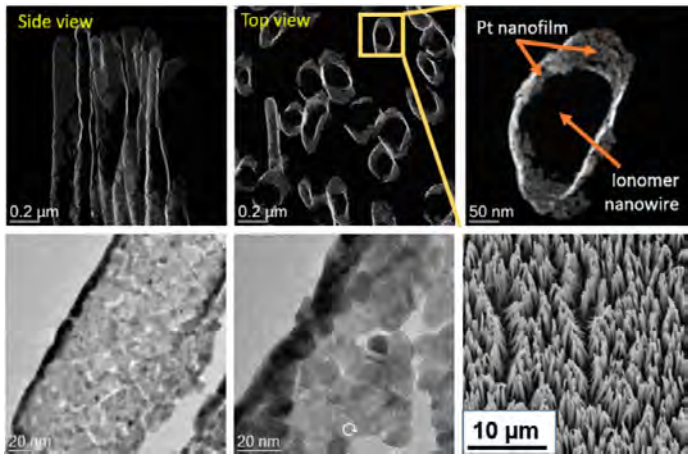
Livache, C., H. Kim, H. Jin, O. Kozlov, I. Fedin and V. I. Klimov. High-Efficiency Photoemission Due to Ultrafast Spin-Exchange Auger Interactions in Mn-Doped CdSe Quantum Dots. Presented at *MRS Spring Meeting 2022*, Honolulu, Hawaii, United States, 2022-05-11 - 2022-05-11. (LA-UR-22-24533)

Touil, A. Quantum Darwinism: the Origin of Objective Classical Reality. . (LA-UR-22-28130)

**Peer-reviewed*

Electrochemical Interfaces Based on Catalytic Nanofilms

Jacob Spendelow
20220372ER



The project team will develop a new type of catalyst based on ultrathin, ultrasmooth 2D films. These nanofilm catalysts are expected to provide higher performance with slower degradation. The team will develop this new catalyst archetype and integrate it into a coaxial nanowire electrodes for fuel cell applications. These catalysts could enable fuel cells with improved efficiency, higher durability, and lower cost.

Project Description

This project will address energy security and clean energy by developing improved catalyst technology for use in fuel cells and related devices. Fuel cells could play a critical role in our clean energy future by enabling carbon-free transportation, and are important for Department of Energy/Energy Efficiency and Renewable Energy programs in this area. Fuel cells also have important applications in sensors and other devices for national security and National Nuclear Security Administration (NNSA) applications. Current fuel cell technology is mainly limited by poor catalytic performance of platinum nanoparticle based cathode catalysts. Expected outcomes of the project include a new type of ultrathin, ultrasmooth platinum nanofilm catalyst with high performance and durability, enabling higher-efficiency fuel cells that are cheaper and more durable, enabling faster deployment in clean energy applications and potentially enabling new NNSA applications.

Publications

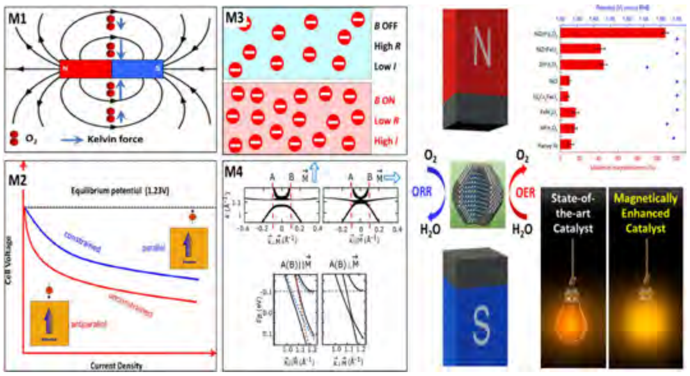
Presentation Slides

Holby, E. F. w22_electrocat Scientific Highlight. . (LA-UR-23-23064)

**Peer-reviewed*

Emergent Phenomena at the Intersection of Magnetism and Catalysis

Xiaojing Wang
20220384ER



Left: This project will build fundamental understanding of emergent phenomena associated with catalysts in magnetic fields by investigating proposed mechanism based on modified electronic structure. Right: Improved understanding of proposed mechanism will enable new catalysts that exploit magnetic enhancement to achieve higher performance and durability.

Project Description

Magnetically-enhanced catalysis could enable transformative improvements in fuel cells and electrolyzers for energy security and National Nuclear Security Administration (NNSA) applications (a rapid growth area for fuel cell research and development at Los Alamos National Laboratory). Studies of emergent phenomena at the intersection of magnetism and catalysis fall under the topic of Complex Functional Materials and Integrated Nanomaterials in the Materials for the Future science pillar. By combining two areas in which Los Alamos has a long history of expertise, magnetic materials and fuel cells/electrolyzers, this project would resolve controversies in the field of magnetic catalysis and generate creative approaches for improved catalysts. This will complement Los Alamos' initiative in Materials for Future as well as the National High Magnetic Field Laboratory's goal to use magnetic fields to understand magnetic phenomena for diverse applications.

Publications

Presentation Slides

Allen, K. J. First principles study of electronic structure and magnetism in CoPt for catalysis. Presented at *T-4 Lightning talks*, Los Alamos, New Mexico, United States, 2022-07-26 - 2022-07-26. (LA-UR-22-27299)

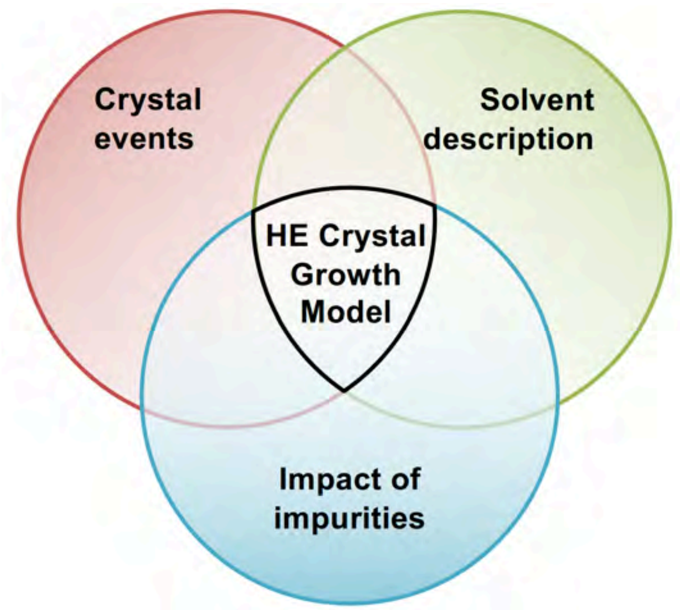
Posters

Allen, K. J., C. A. Lane and J. Zhu. First principles study of electronic structure and magnetism in CoPt for catalysis. Presented at *2022 Annual Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27631)

**Peer-reviewed*

Understanding the Growth Kinetics and Resulting Microstructure in Energetic Materials

Romain Perriot
20220431ER



Building a multi-scale, multi-physics framework of HE crystal growth: The team will use state-of-the-art quantum molecular dynamics (QMD) simulations to compute energetics of crystal events, and devise a kinetic Monte Carlo (KMC) model of HE growth. The model includes the effect of the solvent and impurities, in order to produce a detailed picture of crystal growth.

Project Description

Most practical high explosives (HE) consist of high loading fractions of grains of an energetic molecular crystal in a polymeric binder. The microstructure of these plastic bonded explosives (PBX), which includes factors such as grain size distributions, grain shape, and porosity, largely controls their properties. Many structural factors can adversely affect the safety handling of the materials by increasing sensitivity to explosive initiation. Understanding the growth of organic crystals in general is done essentially through a trial-and-error process, in which parameters such as temperature, and solvent type and concentration, are varied until desired characteristics are obtained. This process of selecting a viable growth path so that we may ultimately obtain the desired PBX microstructure is costly and time consuming, and can expose workers to harsh chemicals that then need to be discarded. In this work, we propose to develop new modeling and simulation capabilities, based on state-of-the-art simulations techniques and validated against experimental data. This framework will allow us to gain a fundamental understanding of the growth processes of HE crystals, and predict optimized growth conditions for known and new forms of HE.

Publications

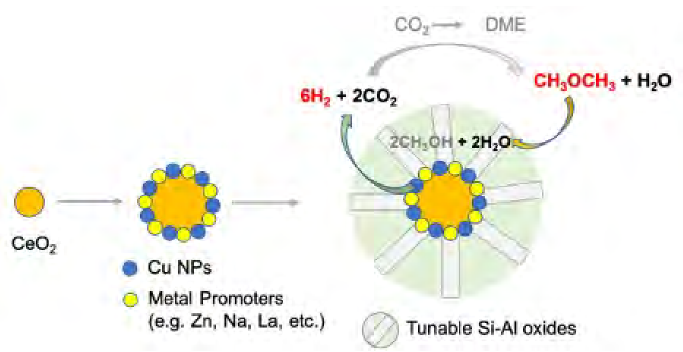
Journal Articles

A. Negre, C. F., A. M. Alvarado, H. Singh, J. D. Finkelstein, E. Martinez Saez and R. T. Perriot. A Methodology to Generate Crystal-based Molecular Structures for Atomistic Simulations. Submitted to *Journal of Physics: Condensed Matter*. (LA-UR-22-29886)

**Peer-reviewed*

Novel Catalyst for Hydrogen (H2) Production from Dimethyl Ether (DME) Steam Reforming

Xiaokun Yang
20220447ER



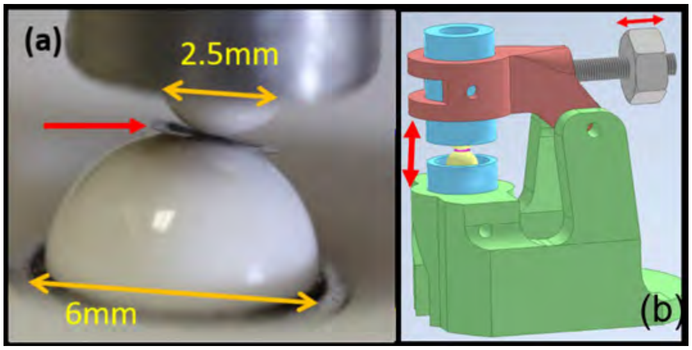
The project proposes to develop a novel acid-tunable hybrid catalyst as micro-reactor. Activity and selectivity will be optimized by tuning the acid site-strength and metal sites in one catalyst. The team will achieve this result by creating a ceria core "acid shell" structure that will also increase the catalyst durability by anchoring the active metal (e.g., Cu) with selected promotors such as Zn, Na, and La.

Project Description

Hydrogen is an important sustainable energy source to diversify our energy portfolio, reduce our dependence on fossil fuels, and address the ever-present climate crisis. This work directly aligns with the Los Alamos National Laboratory 2022 Strategic Implementation Plan priority of energy security. Our goal is to enhance the capability of Dimethyl Ether (DME) to act as a Hydrogen (H2) carrier for fuel cell systems and the auxiliary commercial power market, and reduce the barriers to implementation of DME steam reforming (DME-SR) in commercial applications, and enable new strategy for modern hydrogen economy through developing a fundamental understanding of DME steam reforming mechanisms on heterogeneous catalysts with hybrid functionality. The success of this project will be a game changer not only for the renewable/alternative fuels industry, but more importantly would make DME into a versatile hydrogen carrier allowing for the cost-effective storage and transport of hydrogen. Furthermore, developing downstream hydrogen generation from DME directly aligns with upcoming efforts from Deparment of Energy Hydrogen Fuel Cell Technologies Office (DOE HFTO), Fossil Energy (FE), Vehicle Technologies Office (VTO) and Biomass Energy Technologies Office (BETO) to develop conversion platforms for carbon dioxide (CO2) and related intermediates. DME can be produced from biomass or from CO2 sequestered from industrial point sources or from direct air capture.

Resonant Ultrasound in Thin Films and Mesoscopic Samples: A New Tool to Explore Radiation Damage and Phase Transitions

Boris Maiorov
20220727ER



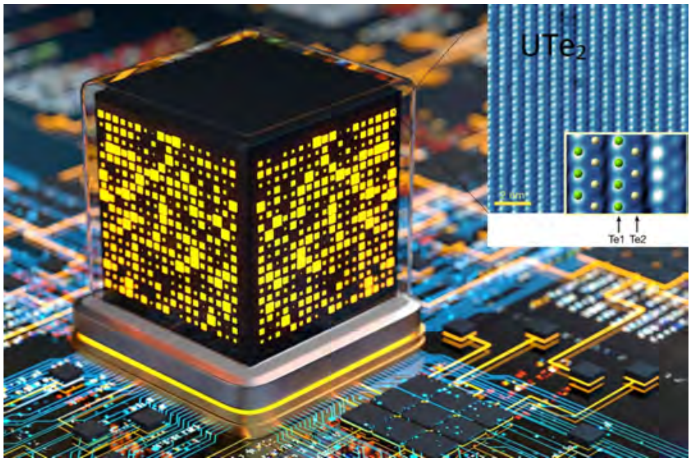
a) Image of a TEM grid held between two piezoelectric transducers in a resonant ultrasound spectroscopy (RUS) experiment. b) Mechanical design of an RUS where the pressure on the sample can be controlled by turning a counterweighted-nut. The pressure regulation allows to maintain the integrity of the sample

Project Description

Elastic moduli are key to understand changes in key materials of interest for National Nuclear Security Administration (NNSA). This proposal answers the needs described in “Materials for the future” to develop novel ways to determine microstructure fingerprints and their changes in extreme environments, e.g. being able to measure all the elastic constants during in-situ irradiation or annealing. Thin films are critical to many applications such as coatings where the damage by irradiation is difficult to observe; if our project succeedss, we will be able to study them with resonant ultrasound spectroscopy for the first time.

Mastering Heavy-Fermion UTe2 Epitaxial Thin Films Synthesis Towards Next Generation Quantum Computers

Aiping Chen
20220728ER



The figure show a future fault-tolerant quantum computer made from topological quantum materials such as UTe2. The inset shows the crystal structure of UTe2. The success of this project is a critical step towards such novel quantum computers, which outperform the current state of the art.

Project Description

Quantum computers have the potential to revolutionize computation by making some classically intractable problems solvable. It is known that current quantum computers based on superconducting qubits suffer from some critical issues. Topological materials have emerged to solve some of these challenges. For example, topological qubits based on the concept of a particle called Majorana fermion, exist in certain topological materials, have been predicted to enable fault-tolerant quantum computation that is can tolerate conventional decoherence sources. However, the challenge is to find quantum materials which host Majorana fermion. Recent reports of chiral spin-triplet superconductivity in uranium detelluride (UTe2) bulk materials indicates that UTe2 could be an ideal system to host Majorana fermion. Developing UTe2 thin film based Josephson junctions is critical to verify Majorana fermion. The outcomes of this project will be developing a new capability of synthesizing high quality UTe2 epitaxial thin films, for the first time. The success of this project will allow Los Alamos National Laboratory to develop UTe2 thin film based Josephson junctions and verify Majorana fermion, a critical step towards quantum computers based on Majorana fermions.

Publications

Journal Articles

Sharma, y., B. Paudel, A. Huon, M. Schneider, P. Roy, Z. Corey, R. Sch\xc3\xb6enemann, A. C. Jones, M. Jaime, D. A. Yarotski, T. Charlton, M. R. Fitzsimmons, Q. Jia, M. T. Pettes, P. Yang and A. Chen. Induced Ferromagnetism in Epitaxial Uranium Dioxide Thin Films. 2022. *Advanced Science*. 2203473. (LA-UR-22-29442 DOI: 10.1002/advs.202203473)

Yu, Z., X. Xu, W. Chen, Y. Sharma, X. Wang, A. Chen, C. Ulmer and A. T. Motta. In-situ irradiation-induced studies of grain growth kinetics of nanocrystalline UO2. Submitted to *Acta Materialia*. (LA-UR-22-27204)

Presentation Slides

Chen, A. Synthesis and Magnetism in Epitaxial Uranium Dioxide Thin Films. Presented at *EMA2023*, Orlando, Florida, United States, 2023-01-17 - 2023-01-21. (LA-UR-23-20447)

Roy, P., A. Chen, H. Zheng and Q. Jia. Anomaly in Hall resistance: Topological Hall effect or two channel anomalous Hall effect?. Presented at *EMA2023*, Orlando, Florida, United States, 2023-01-17 - 2023-01-20. (LA-UR-23-20974)

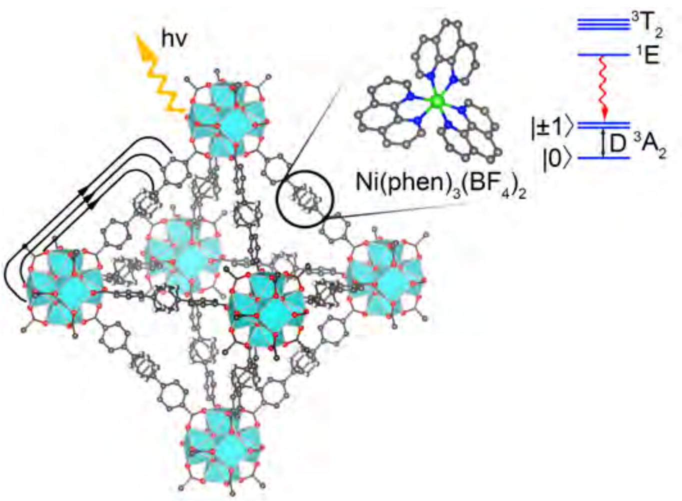
Posters

Roy, P. and A. Chen. Structural, optical and magnetic property of Uranium oxides. Presented at *Second International Workshop on Theory Frontiers in Actinide Science : Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-02-26. (LA-UR-23-22038)

**Peer-reviewed*

Optically Addressable Molecular Qubit Arrays for Quantum Sensing

Ekaterina Dolgopolova
20220744ER



A novel MOF-based magnetic field sensor with incorporated Ni-qubit centers could be a first-time example of molecule-based large scale assemblies capable of quantum sensing with optical read-out and exhibit tunability infeasible with any other types of materials.

Project Description

The advancement in the field of quantum sensing strongly relies on exquisite control over material design and fabrication. In the rapidly growing area of quantum information science, chemical synthesis and framework chemistry are powerful approaches to enable the bottom-up creation of novel modular quantum sensor with tunable properties. The chemistry of metal-organic frameworks (MOFs) – hybrid inorganic-organic porous materials assembled via a molecular-building-block approach – can be used to achieve atomically precise arrangement of identical qubits in scalable networks. Our work will focus on development of novel class of “modular” quantum sensors based on MOFs capable of quantum sensing with optical read-out and exhibit tunability infeasible with any other types of materials.

Publications

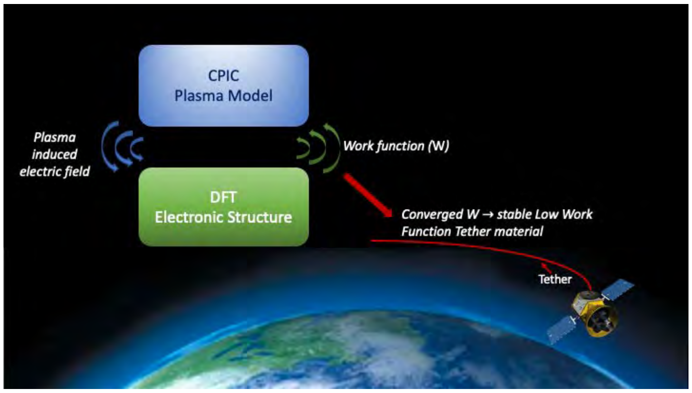
Presentation Slides

Dolgopolova, E. Controlled growth of MOF nanocrystals. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28695)

**Peer-reviewed*

Synergistic Plasma-Material Modeling

Roxanne Tutchton
20220748ER



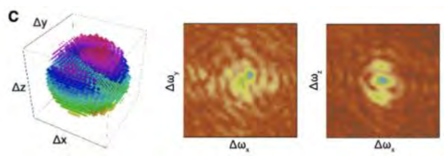
A promising approach to the problem of space debris is the low work function (LWT) tether. We can better understand the impact of a space environment by modeling the effect of plasma on LWT materials. We will design and test a modeling method that couples the LANL developed plasma code, CPIC, with density function theory (DFT) analysis in an iterative loop in order to determine the stability of potential LWT materials in a space environment by calculating a converged work function in the presence of plasma induced electric fields.

Project Description

Space debris is an urgent national security problem which threatens the safe use of space now and in the future, with strong economic and military implications. A promising approach to the problem of space debris is the low work function (LWT) tether. This project will develop new plasma-material interaction capabilities that will support accelerated discovery of surface-engineered materials for tether applications and accelerate a potential solution to the debris problem. Note that these capabilities can also be used for other applications, both in space (minimizing environment impact of spacecraft materials, developing new thrusters for propulsion) and in the laboratory (designing materials resilient to the environment of magnetic fusion energy reactors for energy production). The team's objective is to demonstrate that coupling plasma-material codes for accelerated material discovery for tether applications is possible by predicting materials with stable work functions in a space environment.

Low-Dimensional Latent Space Embedding for Real-Time Three-Dimensional Diffraction Data Analysis

Reeju Pokharel
20220751ER



The image shows the synthetic crystal (left) and corresponding two diffraction patterns (right) of simulated slices of coherent diffraction intensities extracted from a three-dimensional diffraction volume. The synthetic crystal and corresponding diffraction pattern pair forms one of the training set. The project team will be generating 100s of 1000s of such pairs for initial machine learning (ML) model training and testing in this project.

Project Description

Los Alamos National Laboratory heavily utilizes advanced light sources such as the Advanced Photon Source synchrotron and the Linac Coherent Light Source (LCLS) free electron laser for three-dimensional (3D) coherent diffraction imaging (CDI) and high-energy X-ray diffraction microscopy (HEDM) measurements for material science studies and would greatly benefit from a real-time CDI and HEDM reconstruction capabilities as well as an ability to combine the new techniques in which real-time HEDM reconstructions inform the location of CDI measurements to zoom in on material dynamics at nm resolution. Such a real-time capability to guide experiments is desired for Dynamic Mesoscale Materials Science (DMMSC) capabilities for dynamic materials imaging and would place Los Alamos in a leadership role in advanced 3D imaging algorithm development. If successful, the proposed approach will not only benefit Los Almos but also the broader user community that utilizes advanced light sources for understanding materials processing-structure-property relationships.

Publications

Journal Articles

Scheinker, A. and R. Pokharel. Adaptive 3D Autoencoder Latent Space Tuning for Time-Varying Coherent Diffraction Imaging. Submitted to *IEEE Transactions on Image Processing*. (LA-UR-22-30528)

Presentation Slides

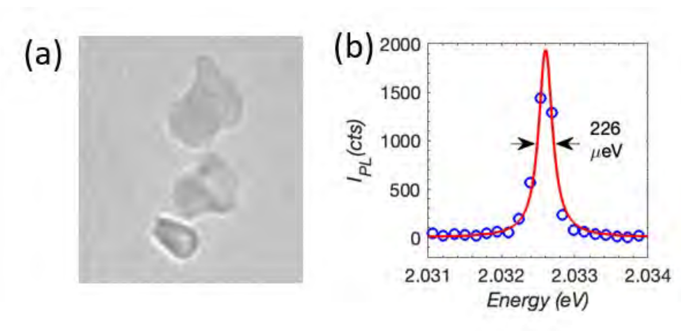
Pokharel, R. Towards machine learning-assisted real-time feedback and guided experiments. Presented at *3DMS 2022*, Washington DC, District Of Columbia, United States, 2022-06-26 - 2022-06-26. (LA-UR-22-26128)

Scheinker, A. and R. Pokharel. Adaptive Latent Space Embedding for Real-Time 3D Diffraction Data Analysis. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-24. (LA-UR-23-23115)

**Peer-reviewed*

Confining Many-body Excitons of Van der Waals Antiferromagents to Nanoscale

Han Htoon
20220757ER



Nanometer size flakes of NiPS3 (a: scanning electron microscope image) are characterized with atomically sharp PL emission peaks (b) at 4 degree K indicating a highly coherent nature of the many-body exciton state. The project team proposed systematic studies toward controlling this many-body exciton states through size and shape of the nanoflakes.

Project Description

Two dimensional atomically thin magnetic materials have recently revealed to foster exciting quantum mechanical collective behaviors that can be exploited for the next generation information processing and sensing technologies. Our preliminary studies on one of such materials, Nickle thiophosphate (NiPS3) has revealed evidence that reducing the size of the crystal to nanometer size (50 x 10 nanometer in diameter and thickness) can have strong influence on manifestation of these quantum mechanical collective behaviors. Here we proposed a series of systematic studies toward understanding physical origin of this effect and exploring nanostructuring as a means to manipulate the quantum mechanical collective behaviors for emergence of new functionalities. This work could open new pathways for development of quantum interfaces allowing exchange of quantum information between superconducting qubits and photons, a critical step for forming a network of quantum computers.

Publications

Presentation Slides

Chandrasekaran, V., C. R. DeLaney, C. A. Lane, J. Zhu, H. Zhao, X. Li, J. A. Hollingsworth, J. D. Watt, A. C. Jones, D. H. Dunlap, A. Piryatinski, S. A. Ivanov and H. Htoon. Magneto-Optical Effects in Nanostructures of van der Waals Antiferromagnet. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22532)

**Peer-reviewed*

Uniaxial Strain-Tuning Quantum States in Actinides

Marcelo Jaime
20220772ER

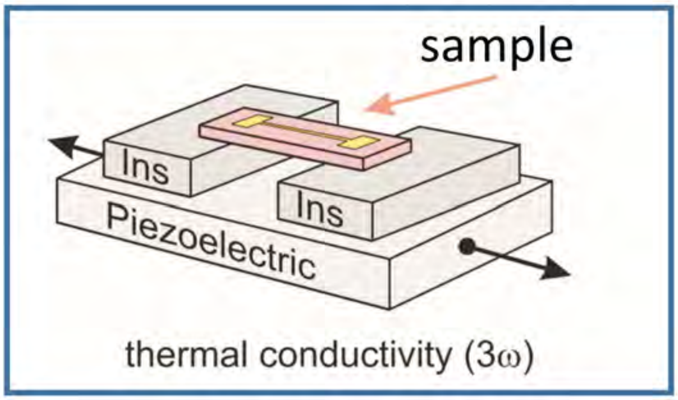


Fig 1. Schematics of the uni-axial strain device that we plan to implement. This includes a sample, onto which a AuGe film is deposited, affixed to insulating posts mounted on a piezoelectric device. When an electric voltage is applied to the piezoelectric material it stretches, straining the sample. Measurements of the electrical resistance of a priorly calibrated AuGe films allows to obtain the sample temperature variations when the base temperature and magnetic field are swept, and the computation of magnetocaloric effect and thermal diffusivity by the 3-omega technique.

Project Description

This project's research addresses the need to better understand the interconnections and correlations between crystal lattice, electronic properties, and magnetism in actinide materials including uranium compounds. Progress in the understanding of these topical and energy-security relevant systems is at the core of the energy security lab strategy on “Advanced materials and systems for clean, efficient transportation and power applications”, and our combined capabilities and expertise are a route to keep Los Alamos at the forefront of the field in a position of leadership.

Publications

Journal Articles

Jaime, M. Crystal Lattice Witness vs. Actor Roles in Correlated Electronic Materials. Submitted to *Journal of the Physical Society of Japan*. (LA-UR-22-26904 DOI: doi.org/https://doi.org/10.7566/JPSJ.91.101005)

Jaime, M., K. Thirunavukkuarasu, G. Radtke, Z. Lu, M. Lazzeri, P. Christianen, M. Ballottin, H. A. Dabkowska, B. D. Gaulin, D. Smirnov and A. Sa\xc3\xbal. Magnetoelastic interactions in SrCu (BO) studied by Raman scattering experiments and first-principles calculations. Submitted to *Physical Review B*. (LA-UR-23-22194)

Jaime, M., Y. Sharma, B. Paudel, A. Huon, M. M. Schneider, P. Roy, Z. Corey, R. U. Schoenemann, A. C. Jones, D. A. Yarotski, T. Charlton, M. Fitzsimmons, Q. Jia, M. T. Pettes, P. Yang and A. Chen. Induced Ferromagnetism in Epitaxial Uranium Dioxide Thin Films. 2022. *Advanced Science*. 2203473. (LA-UR-22-21918 DOI: doi.org/DOI: 10.1002/advs.202203473)

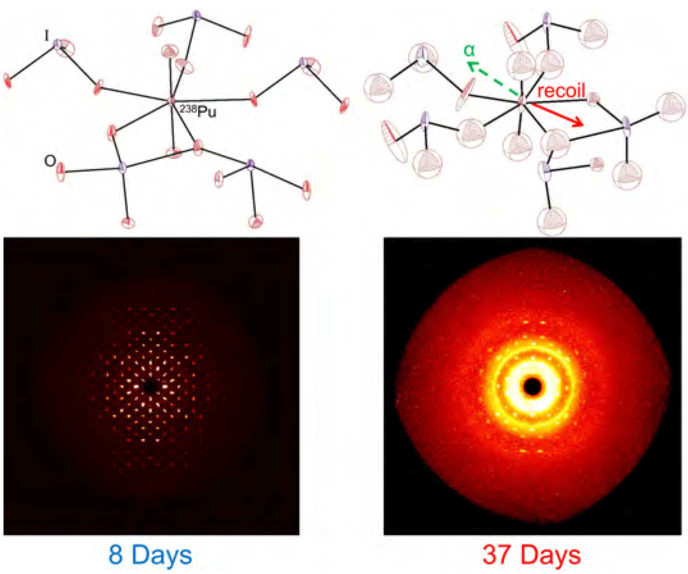
Lee, M., R. U. Schoenemann, H. Zhang, D. Dahlbom, T. Jang, S. Do, A. D. Christianson, S. W. Cheong, J. Park, E. L. Brosha, M. Jaime, K. M. Barros, C. D. Batista and V. Zapf. Field-induced spin level crossings within a quasi-XY antiferromagnetic state in Ba2FeSi2O7. Submitted to *Physical Review B*. (LA-UR-22-31700)

Schoenemann, R. U., P. Rosa, S. M. Thomas, Y. Lai, D. N. Nguyen, J. Singleton, R. D. Mcdonald, V. Zapf and M. Jaime. Thermodynamic evidence for high-field bulk superconductivity in UTe2. Submitted to *Physical Review X*. (LA-UR-22-31567)

**Peer-reviewed*

Accelerated Aging of Crystalline Plutonium Compounds

Justin Cross
20190228ER



Data collected from a sample of plutonyl iodate (PuO2(IO3)2·H2O) enriched with high activity 238Pu demonstrates alpha-induced damage. Top image visualizes average positions of atoms which are typically spheroidal, after accumulating damage these elongate or in the case of O atoms cannot be defined. The x-ray reflections arrayed on the bottom illustrate the loss of crystalline order as the accumulated damage creates an amorphous material. Continued analysis of this and other plutonium compounds elucidate kinetics and mechanisms of decomposition.

Project Description

The goal of this project is to provide experimental data on the aging of well-defined, crystalline plutonium (Pu) salts by spiking 238Pu to produce significant radiation self-damage in a short, yet manageable, period of time. These data can then be used to answer the questions: i. What are the mechanisms of atom displacement and final product formation? ii. How resilient are the selected compounds and how long are they still useful? These results can be integrated into current and future efforts in material disposition, storage, and surveillance. Successful investigations can position the Los Alamos National Labortaory as a leader in radiation damage of Pu compounds. This project will fill a gap of knowledge in the nuclear material management of the entire Department of Energy (DOE) complex as there are no studies on the degradation of crystalline salts with Pu as a main constituent. The findings will have high potential to inform a wide variety of unusual legacy residues that must be handled for future repackaging, storage, and/or disposition. This is especially pertinent with the recent resumption of shipments to the WIPP (Waste Isolation Pilot Plant). State-of-the-art radiological facilities, cutting edge spectroscopy, and access 238Pu place Los Alamos in the unique position to undertake this task.

Technical Outcomes

Experimental data was collected on two different plutonium (Pu) compounds enriched with 238-Pu. This data explicitly shows the stability of tetravalent plutonium (Pu(IV)) versus hexavalent plutonium (Pu(VI) and non-redox active ligands for the intermediate term storage of Pu materials.

Publications

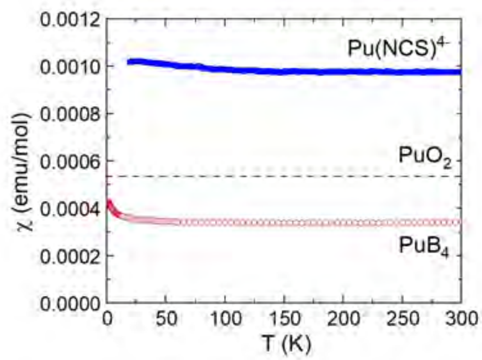
Presentation Slides

Dan, D. Using Metal Organic Frameworks (MOFs) to Quantify the Abundance of Short-Lived Fission Products. . (LA-UR-21-30464)

**Peer-reviewed*

Direct Plutonium-239 Nuclear Magnetic Resonance: A Unique Tool for Understanding Plutonium

Eric Bauer
20200045ER



Plot of magnetic susceptibility vs temperature showing the promising candidate Pu(NCS)^4- , along with measured PuO2, and PuB4 compounds for direct Pu-239 Nuclear Magnetic Resonance (NMR) measurements to establish the Pu-239 chemical shift scale. This scale will lead to an understanding of the bonding and electronic structure of Pu, which is critical to determining the stability of plutonium in waste forms, its reactivity, and migration in the environment.

Project Description

Understanding the chemical bonding of actinide materials is crucial for addressing important issues and finding solutions for problems across the Department of Energy (DOE) Nuclear Complex. Such issues include: controlling chemical processes for nuclear waste remediation and long-term storage, regulating reactivity for efficient actinide separation in reprocessing spent nuclear fuel, and for mitigation of actinide migration in the environment. To advance our understanding of the nature of bonding in the actinides, new spectroscopies must be developed and applied in order to control chemical bonding. We propose to develop of a capability for observing the plutonium-239 (Pu-239) Nuclear Magnetic Resonance signal in a variety of plutonium compounds to understand fundamental issues in actinide chemistry, in particular, bonding and electronic structure to help solve pressing problems facing the Nation.

Technical Outcomes

Los Alamos owns a world-unique direct plutonium-239 nuclear magnetic resonance (NMR) capability. It is a unique and powerful tool for understanding the chemistry of plutonium. The scientific results from this project have significantly increased our understanding of the conditions by which the plutonium-239 NMR signal may be found. This project provided the scientific foundation for the next steps in making direct plutonium-239 NMR an invaluable technique to solve important issues facing the Nation.

Publications

Presentation Slides

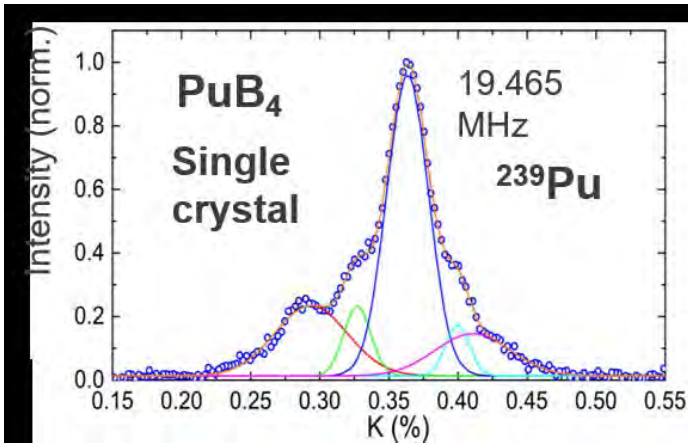
Bauer, E. D., R. Yamamoto, S. B. Blackwell, A. P. Dioguardi, E. G. Bowes, I. D. Piedmonte, S. M. Greer, M. Hirata, S. M. Thomas, T. A. Martinez, C. D. Archuleta, M. Ramos and J. D. Thompson. Nuclear magnetic resonance studies of plutonium compounds. Presented at *Plutonium Futures*, Avignon, France, 2022-09-26 - 2022-09-26. (LA-UR-22-29762)

Dioguardi, A. P., H. Yasuoka, S. M. Thomas, H. Sakai, S. K. Cary, S. A. Kozimor, T. E. Albrecht-Schmitt, H. Choi, J. Zhu, J. D. Thompson, E. D. Bauer and F. Ronning. 239Pu nuclear magnetic resonance in the candidate topological insulator PuB4. Presented at *Plutonium Futures*, Avignon, France, 2022-09-26 - 2022-09-29. (LA-UR-22-29613)

**Peer-reviewed*

Plutonium-239 Nuclear Magnetic Resonance Studies of Aging and Defects

Filip Ronning
20200125ER



This project aims to determine whether plutonium nuclear magnetic resonance (NMR) can provide useful information to study the properties of plutonium-based materials, which degrade as a function of time due to their radioactivity. In the figure, the 239Pu NMR spectra illustrates that at least five unique crystallographic Pu sites exist in our single crystal of PuB4.

Project Description

If successful, this project will result in a local probe of the physical and electronic structure of plutonium-based materials which are continuously evolving as a function of time due to the radioactive decay of plutonium. This could help shed light on the lifetime of the nuclear stockpile as well as with issues of waste storage.

Technical Outcomes

This project illustrated that 239-plutonium nuclear magnetic resonance could be used to observe changes in a materials structure, and dynamical fluctuations caused by the self-radiation damage that occurs in plutonium alloys. This work demonstrated a need to correlate the observed changes to specific metastable defect configurations.

Publications

Journal Articles

*Chiu, W., R. M. Tutchton, G. Resta, T. Lee, E. D. Bauer, F. Ronning, R. T. Scalettar and J. Zhu. Hybridization effect on the X-ray absorption spectra for actinide materials: Application to PuB4. 2020. *Physical Review B*. **102** (8): 085150. (LA-UR-20-21956 DOI: 10.1103/PhysRevB.102.085150)

*Sakai, H., Y. Tokunaga, S. Kambe, J. -. X. Zhu, F. Ronning, J. D. Thompson, S. K. Ramakrishna, A. P. Reyes, K. Suzuki, Y. Oshima and M. Yokoyama. Nano-scale heterogeneity induced by non-magnetic Zn dopants in a quantum critical metal CeCoIn5: 115In NQR/NMR and 59Co NMR Study. 2021. *Physical Review B*. **104** (8): 085106. (LA-UR-21-23885 DOI: 10.1103/PhysRevB.104.085106)

Presentation Slides

Boehm, T. U. Hybridization in the heavy-fermion compound CeRhSn. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22174)

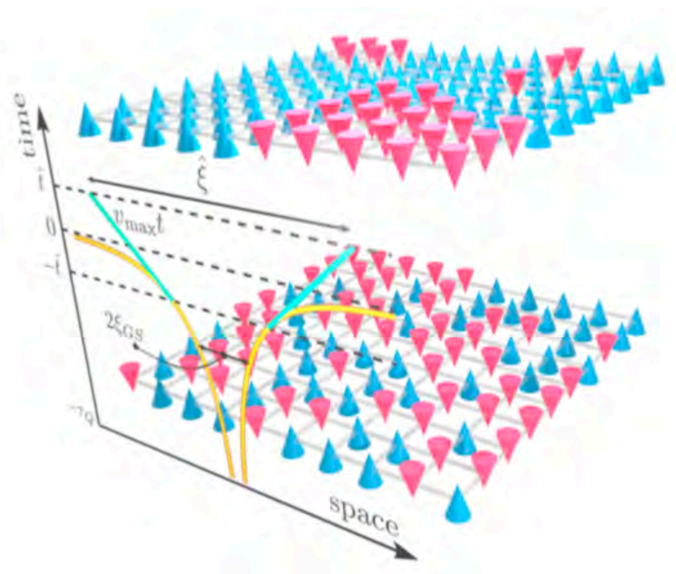
Zhu, J. Hybridization effect on the X-ray absorption spectra for actinide materials. Presented at *Virtual 2020 MRS Spring/Fall Meeting*, Boston, Massachusetts, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-28985)

Zhu, J., W. Chiu, R. M. Tutchton, G. Resta, T. Lee, E. D. Bauer, F. Ronning and R. Scalettar. Hybridization effect on the X-ray absorption spectra for actinide materials: Application to PuB4. Presented at *AVS 67*, Charlotte, North Carolina, United States, 2021-10-25 - 2021-10-28. (LA-UR-21-30174)

**Peer-reviewed*

Dynamics of Quantum Phase Transitions

Wojciech Zurek
20200156ER



The project aims at studying the formation of topological defects in symmetry-breaking phase transitions. The image demonstrates dynamics across a phase transition in a two-dimensional spin-1/2 model. The initial paramagnetic state (bottom) is in general in a coherent superposition, but a measurement of the spin configuration along the ordering direction yields typically a random pattern of spins pointing up or down. After slowly ramping the system across a quantum critical point it develops a quantum superposition of ferromagnetic domains which upon measuring spin configurations along the ordering direction will yield a collapse into domains (top). On the front face -- the growth of the ferromagnetic correlation range as a function of time

Project Description

The project aims at studying the formation of topological defects in symmetry-breaking phase transitions. It is a universal phenomenon relevant for many fields of physics, from cosmology to condensed matter. To achieve this goal we will (theoretically and experimentally) study the dynamics of quantum phase transitions in Bose-Einstein Condensate. The dynamics of quantum phase transitions is a topic that is important to areas of the Laboratory mission ranging from materials to quantum computing. In particular, quantum annealing used by D-Wave is a quantum phase transition. Indeed, the formation of defects during the evolution is a signature of errors in D-Wave. Our research will have an impact on Department of Energy (DOE) missions related to Quantum Information Science (QIS), where consideration is given to both how QIS can benefit DOE's and the Laboratory's Programs, and how Programs can benefit QIS.

Technical Outcomes

New insights into the quantum Kibble-Zurek mechanism include "sonic horizon" view of topological defect formation. Propagation of information in quantum many-body systems was investigated, including decoherence and quantum Darwinism. Numerical simulation of the 2-dimensional quantum Ising phase transition was completed using several numerical methods. Oscillations left behind in the wake of the quantum phase transition was discovered. Oscillations reflects a superposition of different symmetry breaking arrangements and different numbers and locations of topological defects.

Publications

Journal Articles

*Sadhukhan, D., A. Sinha, A. Francuz, J. Stefaniak, M. M. Rams, J. Dziarmaga and W. H. Zurek. Sonic horizons and causality in phase transition dynamics. 2020. *Physical Review B*. **101** (14): 144429. (LA-UR-19-30546 DOI: 10.1103/PhysRevB.101.144429)

Schmitt, M., M. M. Rams, J. P. Dziarmaga, M. Heyl and W. H. Zurek. Quantum phase transition dynamics in the two-dimensional Ising model. Submitted to *Nature Communications*. (LA-UR-21-24924)

*Suzuki, F., M. Lemeshko, W. H. Zurek and R. V. Krems. Anderson Localization of Composite Particles. 2021. *Physical Review Letters*. **127** (16): 160602. (LA-UR-20-28806 DOI: 10.1103/PhysRevLett.127.160602)

*Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. 2022. *Physical Review Letters*. **128** (1): 010401. (LA-UR-21-20437 DOI: 10.1103/PhysRevLett.128.010401)

*Yan, B., V. Y. Chernyak, W. H. Zurek and N. A. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. 2021. *Physical Review Letters*. **126** (7): 070602. (LA-UR-20-26742 DOI: 10.1103/PhysRevLett.126.070602)

Yan, B., W. Chemissany and W. H. Zurek. Quantum Chaos on Complexity Geometry. Submitted to *Physical Review Letters*. (LA-UR-20-22063)

Zurek, W. H. Quantum Theory of the Classical: Einselection, Envariance, and Quantum Darwinism. Submitted to *Entropy*. (LA-UR-21-31822)

Zurek, W. H., A. Touil, B. Yan, D. Girolami and S. Deffner. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Submitted to *Physical Review Letters*. (LA-UR-21-25646)

Zurek, W. H., H. Zeng, C. Zla and H. Zhang. Dynamics of spontaneous symmetry breaking in a holographic superconductor. Submitted to *Nature Physics*. (LA-UR-19-31918)

Zurek, W. H., M. M. Rams and J. Dziarmaga. Coherent Many-Body Oscillations Induced by a Superposition of Broken Symmetry States in the Wake of a Quantum Phase Transition. Submitted to *Physical Review Letters*. (LA-UR-22-20698)

Books/Chapters

Zurek, W. H. Conscious of a Classical World in a Quantum Universe. (LA-UR-20-28307)

Presentation Slides

Girolami, D., A. Touil, B. Yan, S. Deffner and W. H. Zurek. Quantitative limits to quantum correlations in many-body systems: a signature of classical objectivity. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21970)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21968)

Zurek, W. H. Dynamics of Quantum Phase Transitions. . (LA-UR-20-29719)

Zurek, W. H. Information Scrambling, Loschmidt Echo,and Decoherence. . (LA-UR-21-29934)

**Peer-reviewed*

Plutonium Elasticity at Extreme Pressures using Gigahertz Ultrasound in a Diamond Anvil Cell

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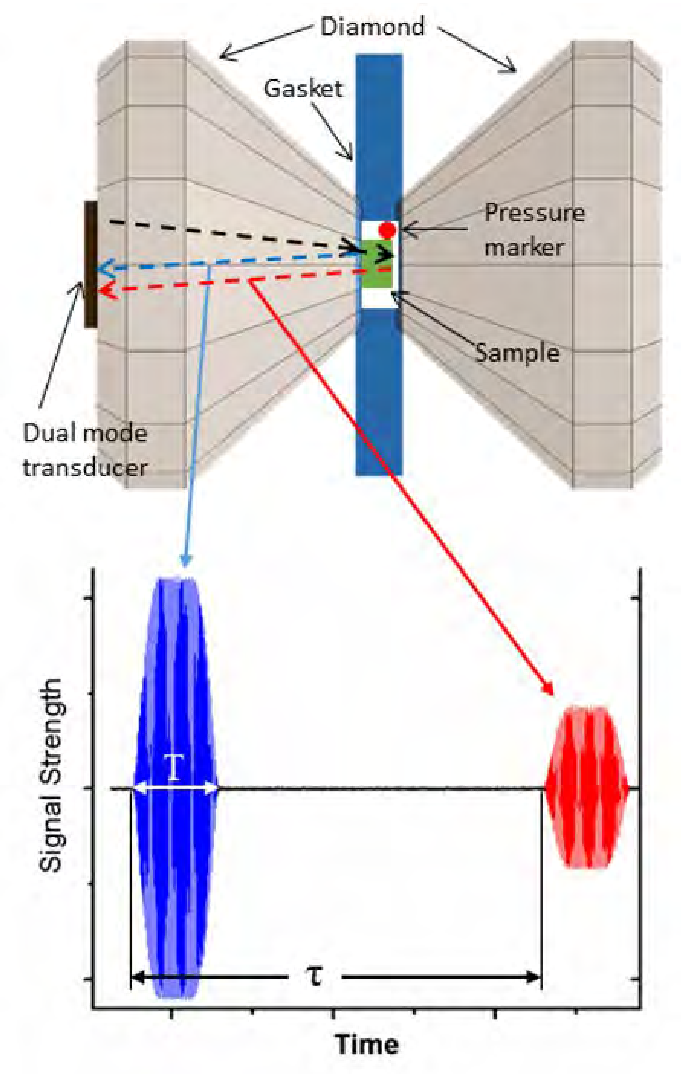

This project is focused on the development of a dual-mode ultrasound transducer fabricated on-diamond (top). The transducer is used to measure the time-of-flight of ultrasound waves (bottom) in the sample which is then used to determine the sound speed and elastic properties of the sample as a function of pressure.

Project Description

Elemental plutonium exhibits one of the most complex phase diagrams in the periodic table. Understanding this phase diagram over a wide range of temperatures and pressures is of critical importance to the Laboratory's mission. Sound velocity and elasticity, which are fundamental thermodynamic properties, play an important role in constraining the equation of state of any material. Capabilities for the direct measurement of sound velocity are currently limited to pressures on the order of 10 gigapascal (GPa). This project will create an institutional capability to directly measure compressional and shear sound velocity simultaneously in a diamond anvil cell, where small samples (0.01 millimeter dimensions) are used to readily achieve pressures in excess of 100 GPa. This unique capability will be achieved by developing a novel dual mode ultra-high frequency acoustic transducer, where "dual-mode," refers to the ability to simultaneously generate shear and compressional acoustic waves. The dual-mode transducers will be designed using finite element methods and fabricated using standard microfabrication techniques. Simultaneous compressional and shear ultrasound measurements on actinide materials at high pressure will constitute successful completion of the project and provide vital information in support of Laboratory and National Nuclear Security Administration (NNSA) missions.

Technical Outcomes

Several important outcomes resulted from the work executed under this project, specifically: 1) the ability to create samples with the correct aspect ratio and roughness for diamond anvil cell experiments; 2) a custom system for generating and recording ultrasound waveforms with gigahertz frequencies; 3) a frequency-domain approach to the analysis of ultrasound data; and 4) significant progress was made toward the microfabrication of gigahertz frequency ultrasound transducers directly on the table of a diamond.

Publications

Presentation Slides

Couper, S. C. Material properties at ultrahigh pressures: developing a gigahertz ultrasound transducer for the diamond anvil cell. Presented at *Agnew and Metropolis Postdoc Fellow Showcase*, Los Alamos, New Mexico, United States, 2022-01-27 - 2022-01-27. (LA-UR-22-20599)

Posters

Couper, S. C. Material properties at ultrahigh pressures: developing a gigahertz ultrasound transducer for the diamond anvil cell. Presented at *Agnew and Metropolis Postdoc Fellow Showcase*, Los Alamos, New Mexico, United States, 2022-01-27 - 2022-01-27. (LA-UR-22-20598)

**Peer-reviewed*

Predicting the Impact Sensitivity of New Explosives through Statistical Modeling

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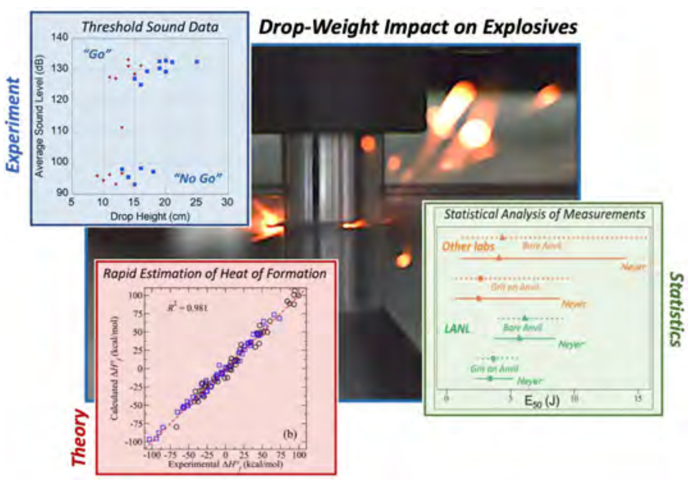

The propensity for explosives to react under normal handling is assessed through a suite of empirical tests, such as the drop-weight impact test, where a 2.5 kilogram mass is dropped onto an explosive that is sandwiched between two anvils. This figure shows the explosive pentaerythritol tetranitrate (PETN), as it initiates in the drop-weight impact test, along with recorded sound levels and statistically analyzed data for hundreds of PETN samples collected at LANL and elsewhere. The project team is currently analyzing thousands of explosives for their impact sensitivity values to identify correlations with important descriptors of their molecular properties.

Project Description

The development of structure-process-performance relationships for the preparation of new energetic materials are crucial to future stewardship of the United States nuclear weapons stockpile, particularly as all future formulations will deviate in some way from those used in historical systems. Therefore, the ability to understand and manipulate the handling safety of new explosives would have a revolutionary effect on applications related to stockpile management, in addition to law enforcement and basic explosives research. Most explosives development is based on a costly trial-and-error approach with rounds of synthesis and testing because we cannot yet predict the properties of new high explosives. Theory and modeling rarely provide clear guidance for the explosive design process, in part because of the multitude of factors that influence handling safety. To address these deficiencies, we will mine historical Laboratory experimental data on high explosive sensitivity testing in order to make an exhaustive search of the properties of explosives that influence sensitivity, and use experimental tests and computational methods to fill in existing gaps in data. Finally, we will use statistical methods to analyze the large quantity of data and derive and validate rules for how to design and screen high explosives for handling safety.

Technical Outcomes

The project utilized state of-the-art atomistic simulations and statistical methods in order to identify multi-variate correlations within the largest dataset of measured explosive impact sensitivity values available. Notably, the statistical analysis of repeat data and the interrelationships between molecular descriptors will allow our scientific community to attach realistic expectations on which data in this field is meaningful, and ultimately will transform how sensitivity data is interpreted in the future.

Publications

Journal Articles

Burch, A. C., H. p. Grennan, D. F. Bahr, J. D. Yeager, M. J. Cawkwell and V. W. Manner. Investigating Correlations Between Explosive Impact Sensitivity and Mechanical Properties Using Nanoindentation. Submitted to *ACS Central Science*. (LA-UR-22-31261)

*Burch, A. C., L. M. Kay, J. D. Yeager, G. W. Brown, B. C. Tappan, M. J. Cawkwell and V. W. Manner. The effect of hardness on polymer-bonded pentaerythritol tetranitrate (PETN) explosive impact sensitivity. 2022. *Journal of Applied Physics*. **131** (1): 015102. (LA-UR-21-29423 DOI: 10.1063/5.0073867)

Cawkwell, M. J., A. C. Burch, J. V. Davis, S. R. Ferreira, N. M. Lease, F. W. I. Marrs and V. W. Manner. Understanding explosive sensitivity with effective trigger linkage kinetics. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-21-32237)

*Cawkwell, M. J., A. C. Burch, S. R. Ferreira, N. Lease and V. W. Manner. Atom Equivalent Energies for the Rapid Estimation of the Heat of Formation of Explosive Molecules from Density Functional Tight Binding Theory. 2021. *Journal of Chemical Information and Modeling*. **61** (7): 3337-3347. (LA-UR-20-21254 DOI: 10.1021/acs.jcim.1c00312)

Cawkwell, M. J., J. V. Davis, N. M. Lease, F. W. I. Marrs, A. C. Burch, S. R. Ferreira and V. W. Manner. Supplementary Material Understanding explosive sensitivity with effective trigger linkage kinetics. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-21-32470)

I. Marrs, F. W., J. V. Davis, A. C. Burch, G. W. Brown, N. M. Lease, P. L. Huestis, M. J. Cawkwell and V. W. Manner. Chemical predictors for a large-scale study on drop-weight impact sensitivity of high explosives. Submitted to *ACS Central Science*. (LA-UR-22-25745)

*Marrs, F. W., V. W. Manner, A. C. Burch, J. D. Yeager, G. W. Brown, L. M. Kay, R. T. Buckley, C. M. Anderson-Cook and M. J. Cawkwell. Sources of Variation in Drop-Weight Impact Sensitivity Testing of the Explosive Pentaerythritol Tetranitrate. 2021. *Industrial & Engineering Chemistry Research*. **60** (13): 5024-5033. (LA-UR-20-30351 DOI: 10.1021/acs.iecr.0c06294)

Books/Chapters

Cawkwell, M. J., S. R. Ferreira, N. M. Lease and V. W. Manner. Ranking explosive sensitivity with chemical kinetics derived from molecular dynamics simulations. (LA-UR-20-26693)

Presentation Slides

Burch, A. C., F. W. I. Marrs, J. V. Davis, J. D. Yeager, M. J. Cawkwell and V. W. Manner. Statistical analysis of large data sets to improve understanding of explosive sensitivity. Presented at *JANNAF*, online, New Mexico, United States, 2021-12-06 - 2021-12-16. (LA-UR-21-31580)

Burch, A. C., H. P. Grennan, D. F. Bahr, J. D. Yeager, M. J. Cawkwell and V. W. Manner. Investigating correlations between explosive impact sensitivity and mechanical properties using nanoindentation. Presented at *Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-25495)

Cawkwell, M. J. Institutional computing report: w21_latte_qmd. . (LA-UR-22-24550)

Cawkwell, M. J., J. V. Davis, N. M. Lease, F. W. I. Marrs, A. C. Burch, S. R. Ferreira and V. W. Manner. Model for explosive sensitivity using enthalpy of explosion and effective trigger linkage kinetics. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-25729)

Davis, J. V., F. W. I. Marrs, A. C. Burch, N. M. Lease, S. R. Ferreira, M. J. Cawkwell and V. W. Manner. A Bond Centered Approach to Energetic Performance and Sensitivity. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26006)

Manner, V. W. Hazard Analyses in Explosives Research and Career Paths. Presented at *Yale Chemistry Joint Safety Team and Professional Development Network*, New Haven, Connecticut, United States, 2021-05-14 - 2021-05-14. (LA-UR-21-24574)

I. Marrs, F. W. Influence networks in longitudinal bipartite relational data. Presented at *Joint Statistical Meetings*, Virtual, New Mexico, United States, 2021-08-08 - 2021-08-12. (LA-UR-21-26739)

I. Marrs, F. W., J. V. Davis, A. C. Burch, G. W. Brown, N. M. Lease, P. L. Huestis, M. J. Cawkwell and V. W. Manner. Chemical determinants of drop-weight impact sensitivity in high explosives. Presented at *APS Shock Compression of Condensed Matter Conference*, Anaheim, California, United States, 2022-07-10 - 2022-07-15. (LA-UR-22-25737)

**Peer-reviewed*

Shedding Light on Quantum Phenomena in Topological Chiral Crystals

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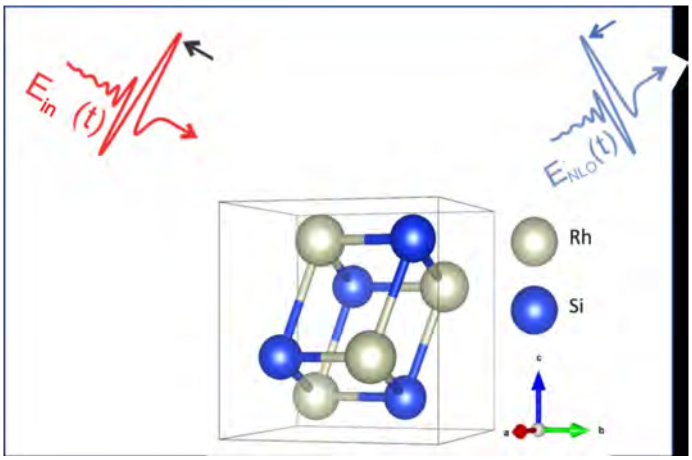

This project aims to use light to reveal topological quantum phenomena in chiral crystals, confirming theoretical predictions and providing new insight into these fascinating materials. The figure demonstrates nonlinear optics, in which an intense, ultrashort optical pulse (red) interacts with a material to generate an output pulse at a different frequency (blue), is a powerful probe of materials. Theoretical work has shown that nonlinear optics can be used to probe quantum effects in topological materials, thus providing new insight into their properties.

Project Description

Within the past decade, topological materials have gone from an exotic curiosity to the subject of the 2016 Nobel Prize in Physics. Topological semimetals (TSMs) in particular exhibit a host of striking phenomena, giving them great promise for applications including quantum computing, quantum information, and spintronics. However, despite the intense effort in this burgeoning area, it has been hard to measure clear-cut signatures of material topology. This in turn has prevented these unique materials from realizing their vast potential for novel applications. Topological chiral crystals (TCCs) are a new class of materials with substantially improved properties that make measurements of previously elusive topological phenomena possible. Optical experiments can provide clear signatures of these phenomena, putting us in an excellent position to apply our extensive expertise in optical measurements on TSMs to TCCs. Our chief innovation is thus to combine our expertise in optical studies of TSMs with the availability of newly developed topological chiral crystals to clearly reveal signatures of topology. Our studies will thus establish the unique character of these systems, providing long awaited insight and comparison to theoretical predictions that sets the stage for future studies and applications of these fascinating materials.

Technical Outcomes

Nonlinear optical phenomena in topological semimetals was successfully investigated in this project, where the team has discovered a novel means to manipulate electronic symmetry in this class of materials. Combined with theoretical insights, these findings open the door for translational research, which can directly build on the success of this project.

Publications

Journal Articles

Chen, L., C. Setty, H. Hu, M. G. Vergniory, S. E. Grefe, A. Prokofiev, S. Paschen, J. Cano and Q. Si. Topological Semimetal driven by Strong Correlations and Crystalline Symmetry. Submitted to *Nature Physics*. (LA-UR-21-28235)

Grefe, S. E., Q. Si, H. Lai and S. Paschen. Extreme response of Weyl-Kondo semimetal to Zeeman coupling. Submitted to *Physical Review Letters*. (LA-UR-20-30516)

*Krapivin, V., M. Gu, D. Hickox-Young, S. W. Teitelbaum, Y. Huang, G. de la Pena, D. Zhu, N. Sirica, M. -. Lee, R. P. Prasankumar, A. A. Maznev, K. A. Nelson, M. Chollet, J. M. Rondinelli, D. A. Reis and M. Trigo. Ultrafast Suppression of the Ferroelectric Instability in. 2022. *Physical Review Letters*. **129** (12): 127601. (LA-UR-22-30598 DOI: 10.1103/PhysRevLett.129.127601)

*Lee, M., N. Sirica, S. W. Teitelbaum, A. Maznev, T. Pezeril, R. Tutchton, V. Krapivin, G. A. de la Pena, Y. Huang, L. X. Zhao, G. F. Chen, B. Xu, R. Yang, J. Shi, J. -. Zhu, D. A. Yarotski, X. G. Qiu, K. A. Nelson, M. Trigo, D. A. Reis and R. P. Prasankumar. Direct Observation of Coherent Longitudinal and Shear Acoustic Phonons in TaAs Using Ultrafast X-Ray Diffraction. 2022. *Physical Review Letters*. **128** (15): 155301. (LA-UR-20-29013 DOI: 10.1103/PhysRevLett.128.155301)

Sirica, N. S. and R. P. Prasankumar. Shaking up topology with light. Submitted to *Nature Materials*. (LA-UR-21-20965)

*Sirica, N., P. P. Orth, M. S. Scheurer, Y. M. Dai, M. -. C. Lee, P. Padmanabhan, L. T. Mix, S. W. Teitelbaum, M. Trigo, L. X. Zhao, G. F. Chen, B. Xu, R. Yang, B. Shen, C. Hu, C. -. C. Lee, H. Lin, T. A. Cochran, S. A. Trugman, J. -. X. Zhu, M. Z. Hasan, N. Ni, X. G. Qiu, A. J. Taylor, D. A. Yarotski and R. P. Prasankumar. Photocurrent-driven transient symmetry breaking in the Weyl semimetal TaAs. 2022. *Nature Materials*. **21** (1): 62-66. (LA-UR-20-23580 DOI: 10.1038/s41563-021-01126-9)

Presentation Slides

Grefe, S. E. Strongly correlated topological semimetals. Presented at *Electronic topology across the correlation spectrum*, Aspen, Colorado, United States, 2021-07-12 - 2021-07-30. (LA-UR-21-27196)

Grefe, S. E. The Weyl Kondo Semimetal. Presented at *Topological Materials: from weak to strong correlations - online 'stay in touch' meeting*, Online/Virtual, New Mexico, United States, 2021-08-04 - 2021-08-06. (LA-UR-21-27751)

Grefe, S. E. Extreme topological tunability of Weyl-Kondo semimetal to Zeeman coupling. Presented at *Part II - RCQM Workshop on Topological Materials and Electron Correlations*, Houston, Texas, United States, 2021-11-15 - 2021-11-17. (LA-UR-21-31390)

Grefe, S. E. Weyl-Kondo semimetal: Extreme topological tunability and nonlinear optical exploration. Presented at *American Physical Society (APS) March Meeting*, Virtual/Online, New Mexico, United States, 2022-03-13 - 2022-03-18. (LA-UR-22-22432)

Grefe, S. E. The Weyl-Kondo semimetal: high-harmonic generation and extreme topological tunability. Presented at *International Conference on Strongly Correlated Electron Systems*, Amsterdam, Netherlands, 2022-07-24 - 2022-07-29. (LA-UR-22-27832)

Grefe, S. E., H. Lai, S. Paschen and Q. Si. Extreme response of Weyl-Kondo semimetal to Zeeman coupling. Presented at *2021 American Physical Society March Meeting (Virtual/Online)*, Virtual/Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22720)

Grefe, S. E., R. P. Prasankumar, Q. Si and J. Zhu. High harmonic generation in Weyl-Kondo semimetals. Presented at *2021 American Physical Society March Meeting (Virtual/Online)*, Online/Virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22719)

Grefe, S. E., S. Paschen, Q. Si and J. Zhu. Weyl-Kondo semimetals: extreme topological tunability and nonlinear optical signatures. Presented at *Strongly correlated electron systems 2020/21*, Online/Virtual, New Mexico, United States, 2021-09-27 - 2021-10-01. (LA-UR-21-29633)

Posters

Grefe, S. E. and J. Zhu. High-harmonic generation in a Weyl-Kondo semimetal. Presented at *Photoinduced Phase Transitions and Cooperative Phenomena*, Online/Virtual, New Mexico, United States, 2021-11-08 - 2021-11-19. (LA-UR-21-31211)

Sirica, N. S., P. Orth, M. Scheurer, R. Tobey, Y. Dai, M. C. Lee, P. Padmanabhan, L. M. T. Mix, S. Tietelbaum, M. Trigo, L. Zhao, G. Chen, B. Xu, R. Yang, B. Shen, C. Hu, C. C. Lee, L. Hsin, T. Cochran, P. R. Bowlan, A. K. Azad, S. A. Trugman, J. Zhu, M. Z. Hazan, N. Ni, X. Qiu, A. J. Taylor, D. A. Yarotski and R. P. Prasankumar. MANIPULATING ELECTRONIC SYMMETRY IN THE WEYL SEMIMETAL TaAs USING ULTRAFAST PHOTOCURRENTS. Presented at *CATS EFRC PI Meeting*, Ames, Iowa, United States, 2021-09-27 - 2021-09-27. (LA-UR-21-29519)

Other

Sirica, N. S., R. Y. Zhu, D. A. Yarotski and M. C. Lee. Optical pump-probe data on Weyl semimetals. Dataset. (LA-UR-20-24079)

**Peer-reviewed*

Transition Metal Nitrides for Efficient Nitrogen Electrocatalysis

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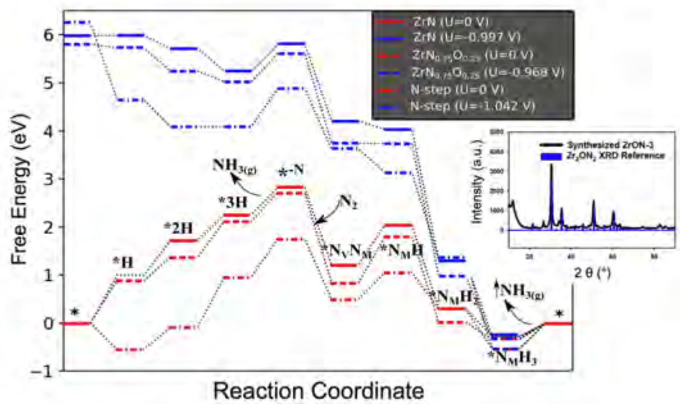

This LDRD-funded exploratory research is investigating oxynitride materials for their potential towards electrochemical nitrogen reduction reaction (NRR). The calculated energy barriers for the various individual elementary reactions of the NRR on zirconium nitride (ZrN) and zirconium oxynitride (ZrOxNy) surfaces with and without surface-steps is illustrated here. The calculations show that the nitrogen vacancy formation is the rate limiting step for NRR and can be lower in oxynitrides and surfaces with steps. Inset: The x-ray powder diffraction (XRD) pattern of the experimentally prepared ZrOxNy with a reference pattern showing the match.

Project Description

Nitrogen reduction reaction (NRR) to produce ammonia by the Haber-Bosch (HB) process is leaving a significant carbon footprint and accounts for ~2% of global natural gas consumption and ~3% of greenhouse gas emissions. The electrochemical production of ammonia would not only solve this problem but also provide an additional way to store the energy from intermittent renewable electricity in a feedstock/fuel. The major challenge here is finding an effective catalyst for NRR since conventional precious metal-based catalysts suffer from competing hydrogen evolution reaction and catalysts with adequate selectivity have not been discovered. In this regard, transition metal nitrides (TMNs) have many advantages over metal catalysts as ammonia formation reaction occurs between the nitrogen on the nitride and adsorbed hydrogen, removing the need for pre nitrogen adsorption on the catalyst surface. We aim to prepare a variety of transition metal nitrides and evaluate their catalytic activity towards NRR in both aqueous and non-aqueous electrolytes. We will also develop the theoretical understanding of the NRR mechanism in these TMNs and develop design principles for the synthesis of efficient NRR catalysts.

Technical Outcomes

The team synthesized, characterized, and electrochemically tested novel Molybdenum carbide and Zirconium oxynitride model systems for Nitrogen Reduction Reaction (NRR) activity in water. Electrochemical NRR testing resulted in rigorous testing conditions to confirm NRR activity were developed and implemented. Additionally, theoretical counterparts established model systems to understand the NRR mechanism at the proposed material surfaces. Further high throughput computational screening for stable oxynitride perovskites successfully identified 295 potentially novel and stable compounds as future targets.

Publications

Journal Articles

*Roads less traveled: Nitrogen reduction reaction catalyst design strategies for improved selectivity. 2021. *Current Opinion in Electrochemistry*. **28**: 100723. (LA-UR-20-25145 DOI: 10.1016/j.coelec.2021.100723)

Banerjee, A., B. M. Ceballos, C. Kreller, R. Mukundan and G. Pilania. A First Principles Investigation of Nitrogen Reduction to Ammonia on Zirconium Nitride and Oxynitride Surfaces. Submitted to *Journal of Materials Science*. (LA-UR-21-29531)

*Young, S. D., A. Banerjee, G. Pilania and B. R. Goldsmith. Perovskite oxynitrides as tunable materials for electrocatalytic nitrogen reduction to ammonia. 2021. *Trends in Chemistry*. **3** (9): 694-696. (LA-UR-21-26260 DOI: 10.1016/j.trechm.2021.07.002)

Young, S., B. M. Ceballos, A. Banerjee, R. Mukundan, G. Pilania and B. R. Goldsmith. Metal Oxynitrides for the Electrocatalytic Reduction of Nitrogen to Ammonia. Submitted to *Journal of Physical Chemistry C*. (LA-UR-22-27402)

Posters

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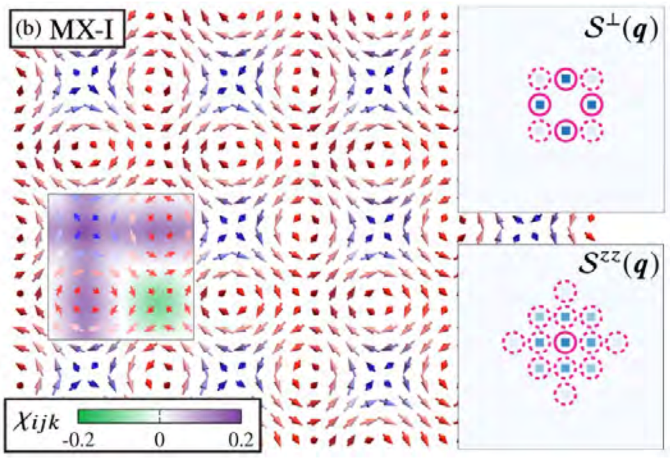
**Peer-reviewed*

Design Principles for Skyrmions in Fluorine-Electron Materials

Shizeng Lin
20200357ER



Spin configurations of the double-Q states. The insets show the in-plane and out-of-plane static spin structure factors in the first Brillouin zone (the intensities are colored in log scale). On the left part of each panel, the team has also colored the scalar chirality in the magnetic unit cell.

Project Description

Skyrmions are particle-like objects stabilized in magnets. They are promising candidates for next-generation memory devices. It is desirable to expand the skyrmion-materials in order to optimize skyrmion properties. This research will reveal a novel mechanism for skyrmion stabilization in fluorine (f)-electron materials. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion materials and spintronics.

Technical Outcomes

The project team clearly demonstrated an extremely rich spin texture in f-electron materials, which are promising for applications in novel devices, such as next-generation magnetic memories. Starting from the current successful project, the team will continue investigating the rich physics in f-electron materials, where the conduction electrons and magnetic moments conspire to stabilize varieties of quantum states.

Publications

Journal Articles

Arachchige, H. S., L. M. DeBeer-Schmitt, L. L. Kish, B. K. Rai, A. F. May, D. S. Parker, G. Pokharel, W. Tian, D. G. Mandrus, M. Bleuel, Z. Islam, G. Fabbris, H. X. Li, S. Gao, H. Miao, S. M. Thomas, P. Rosa, J. D. Thompson, S. Lin and A. D. Christianson. Nanometric modulations of the magnetic structure of the element Nd. Submitted to *Physical Review Research*. (LA-UR-22-27782)

Banerjee, S., U. Kumar and S. Lin. Inverse Faraday effect in Mott insulators. Submitted to *Physical Review Letters*. (LA-UR-21-28801)

Banerjee, S. and S. Lin. Emergent orbital magnetization in Kitaev quantum magnets. Submitted to *Physical Review X*. (LA-UR-22-28455)

Bordelon, M. M., C. Girod, F. Ronning, K. Rubi, N. Harrison, J. D. Thompson, C. Dela Cruz, S. M. Thomas, E. D. Bauer and P. F. S. Rosa. Interwoven atypical quantum states in CeLiBi2. 2022. *Physical Review B*. **106** (21): 214433. (LA-UR-22-30685 DOI: 10.1103/PhysRevB.106.214433)

Huang, C. L., N. Wei, I. Blinov, W. Qin, A. MacDonald and T. Wolf. Spin and Orbital Metallic Magnetism in Rhombohedral Trilayer Graphene. Submitted to *Physical Review Letters*. (LA-UR-22-22867)

Huang, C. L., N. Wei, T. Wolf, W. Qin, I. Blinov and A. MacDonald. Functional Renormalization Group Study of Superconductivity in Rhombohedral Trilayer Graphene. Submitted to *Physical Review Letters*. (LA-UR-22-22744)

Jeong, J., S. Lin, Y. Lee, C. Lee, J. W. Choi, Y. H. Jeong, H. J. Chang and J. Kim. Hard skyrmions in a rare earth permanent magnet. Submitted to *Nature Communications*. (LA-UR-19-31929)

*Kumar, U., S. Banerjee and S. Lin. Floquet engineering of Kitaev quantum magnets. 2022. *Communications Physics*. **5** (1): 157. (LA-UR-21-30565 DOI: 10.1038/s42005-022-00931-1)

Li, Z., J. Su, S. Lin, D. Liu, Y. Gao, S. Wang, H. Wei, T. Zhao, Y. Zhang, C. Jianwang and B. G. Shen. Field-free magnetic topology transformation in the domain wall of ferrimagnetic GdFeCo. Submitted to *Nature Nanotechnology*. (LA-UR-20-27806)

Lin, S. Skyrmion lattice in centrosymmetric magnets with local Dzyaloshinsky-Moriya interaction. Submitted to *Scipost Physics*. (LA-UR-21-32483)

Rostami, H., S. Banerjee, G. Aeppli and A. V. Balatsky. Instabilities of Dirac fermions induced by singular interactions. Submitted to *Annals of Physics*. (LA-UR-22-23341)

Seo, S., S. Hayami, Y. Su, S. M. Thomas, F. Ronning, E. D. Bauer, J. D. Thompson, S. Lin and P. Ferrari Silveira Rosa. Spin-texture-driven electrical transport in multi-Q antiferromagnets. Submitted to *Nature Communications*. (LA-UR-20-24023)

Wang, Z., H. Zhou, M. Guo, L. Zhao, T. Xu, Y. Dong, K. Wu, S. G. Je, W. Chao, M. Im, H. Han, S. Lee, K. Lee, C. Song, H. Wu, S. Lin and W. Jiang. Thermal generation, manipulation and detection of skyrmions. Submitted to *Nature Electronics*. (LA-UR-19-25918)

*Wang, Z., Y. Su, S. Lin and C. D. Batista. Skyrmion Crystal from RKKY Interaction Mediated by 2D Electron Gas. 2020. *Physical Review Letters*. **124** (20): 207201. (LA-UR-19-31876 DOI: 10.1103/PhysRevLett.124.207201)

Zhao, X., J. Tang, K. Pei, W. Wang, S. Lin, H. Du, M. Tian and R. Che. Deterministic generation of skyrmions and antiskyrmions by electric current. Submitted to *Nature Nanotechnology*. (LA-UR-21-20900)

*Zhentao, W., S. Ying, L. Shi-Zeng and C. D. Batista. Meron, skyrmion, and vortex crystals in centrosymmetric tetragonal magnets. 2021. *Physical Review B*. **103** (10): 104408. (LA-UR-20-29175 DOI: 10.1103/PhysRevB.103.104408)

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Saxena, A. B. Hopfions in Anisotropic Heisenberg Magnets. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-14. (LA-UR-22-21627)

Saxena, A. B. Non-Hermitian Qubits and Photonic Lattices. . (LA-UR-22-23542)

Saxena, A. B., R. Balakrishnan and R. Dandoloff. Topological Defects in Ferroelectrics and Functional Materials. Presented at *American Ceramic Society (PACC-FMA) 2022*, Panama City, Panama, 2022-07-24 - 2022-07-24. (LA-UR-22-27281)

Posters

Lin, S. Topological spin texture in centrosymmetric magnets. Presented at *VI International Workshop Dzyaloshinskii-Moriya Interaction and Exotic Spin Structures*, Vyborg, Russia, 2021-09-06 - 2021-09-06. (LA-UR-21-28964)

Zhu, J., A. Ghosh and S. Lin. Data-driven study of magnetic interactions of transition-metal based 2D materials. Presented at *2020 APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-19-30770)

**Peer-reviewed*

Pushing Past the 100 Tesla Threshold: Designing a High Conductivity/High Strength Metallic Composite Conductor

John Carpenter
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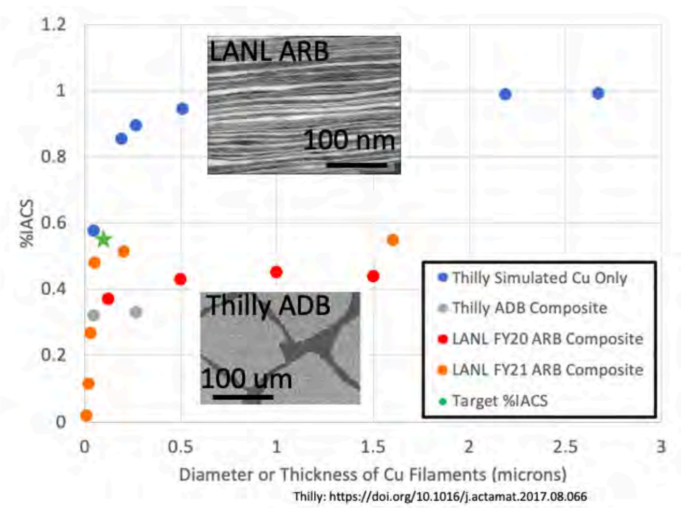

Plot comparing conductivity normalized for highly conductive Cu (IACS %) as a function of filament size (accumulative drawing and bonded material [ADB]) and layer thickness (accumulative roll bonding [ARB]). Magnet material researcher Thilly's reported results for ADB represent the currently used, state-of-the-art for magnet material design and conductivity. Material developed in FY20/21 at LANL using ARB (red and orange symbols, respectively) is showing improvements in conductivity for similar microstructural length scales. When coupled with high strength (not shown), this project is producing material with improved strength and conductivity to enable 120T high field pulsed magnets for actinide and superconductivity research.

Project Description

Energy security is of critical interest to the Department of Energy (DOE) and is one of the three main missions for Los Alamos National Laboratory. This project will develop a new metallic nanocomposite material that will enable an increase in the upper limit of magnetic fields of 100 Tesla (T) to 120 T. Currently magnetic fields are used to characterize or look at a wide variety of energy related materials such as high temperature superconductors. For the case of high temperature superconductive materials, the underlying mechanism of electron pairing remains unknown although decades have passed since the discovery of this phenomenon. Currently, we lack magnetic fields sufficient to suppress superconductivity for the materials in which the pairing is strongest. Magnetic fields beyond 100 T would enable study of the pairing interaction that is essential for development of future high temperature superconducting materials. Understanding this phase transition would enable development of near-room-temperature superconductive materials that would reinvent our current energy grid. This reinvention would be enabled by removing the resistance in the power lines that transition power from plants to homes. This increases efficiency of distribution for all power sources from wind to nuclear to coal.

Technical Outcomes

Consistent with modeling results from this project, conductivity was largely unaffected by microstructure or strength at the nanometer scale layer thicknesses. This drove the processing towards volume fraction manipulation which helped increase the conductivity up from 40% to 60% with minimal decreases in strength. This exhibited the power of the new conductivity-strength modeling framework developed in this project with processing of highly conductive nanolamellar composites.

Publications

Journal Articles

*Blaschke, D. N., C. Miller, R. Mier, C. Osborn, S. M. Thomas, E. L. Tegtmeier, W. P. Winter, J. S. Carpenter and A. Hunter. Predicting electrical conductivity in Cu/Nb composites: A combined model-experiment study. 2022. *Journal of Applied Physics*. **132** (4): 45105. (LA-UR-21-30714 DOI: 10.1063/5.0096880)

*Blaschke, D. N., C. Miller, R. Mier, C. Osborn, S. M. Thomas, E. L. Tegtmeier, W. P. Winter, J. S. Carpenter and A. Hunter. Predicting electrical conductivity in Cu/Nb composites: A combined model-experiment study. 2022. *Journal of Applied Physics*. **132** (4): 45105. (LA-UR-21-30714 DOI: 10.1063/5.0096880)

*Blaschke, D. N., C. Miller, R. Mier, C. Osborn, S. M. Thomas, E. L. Tegtmeier, W. P. Winter, J. S. Carpenter and A. Hunter. Predicting electrical conductivity in Cu/Nb composites: A combined model-experiment study. 2022. *Journal of Applied Physics*. **132** (4): 45105. (LA-UR-21-30714 DOI: 10.1063/5.0096880)

Blaschke, D. and A. Hunter. Predicting electrical conductivity in bi-metal composites. Submitted to *TBD*. (LA-UR-22-29552)

Carpenter, J. S., C. Miller, D. Blaschke, W. P. I. Winter and S. M. Thomas. Optimizing Conductivity and Hardness in Cu-Nb Nanolamellar Composites Fabricated through Accumulative Roll Bonding Without Intermittent Heat Treatments. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-23-20261)

*Carpenter, J. S., C. Miller, D. J. Savage, D. R. Coughlin, E. L. Tegtmeier and W. P. Winter. The Impact of Rolling at Temperature on Conductivity and Texture in Nanolamellar Cu/Nb Bimetallic Composites. 2022. *Metallurgical and Materials Transactions A*. **53** (6): 2208-2213. (LA-UR-21-31438 DOI: 10.1007/s11661-022-06662-w)

Carpenter, J. S., D. J. Savage, C. Miller, R. J. Mccabe, S. Zheng, D. R. Coughlin and S. C. Vogel. Accumulative Roll Bonding of Alloy 2205 Duplex Steel and the Accompanying Impacts on Microstructure, Texture, and Mechanical Properties. 2023. *Metallurgical and Materials Transactions A*. **54** (2): 537-548. (LA-UR-22-22594 DOI: 10.1007/s11661-022-06897-7)

Cheng, J. Y., M. Radhakrishnan, C. Miller, R. M. Mier, S. C. Vogel, J. S. Carpenter, O. Anderoglu and N. A. Mara. The Influence of Thermomechanical Treatment Pathways on Texture and Mechanical Properties in ARB Cu/Nb Nanolaminates. Submitted to *Materials Science and Engineering A*. (LA-UR-22-29079)

*Ma, X., B. Gwalani, J. Tao, M. Efe, M. Olszta, M. Song, S. Yadav, A. Yu, T. J. Nizolek, J. S. Carpenter, B. Zhou, A. Devaraj, S. Mathaudhu and A. Rohatgi. Shear strain gradient in Cu/Nb nanolaminates: Strain accommodation and chemical mixing. 2022. *Acta Materialia*. **234**: 117986. (LA-UR-21-31147 DOI: 10.1016/j.actamat.2022.117986)

*H. A. *. B. I. J. *. L. R. A. *. D. K. *. M. E. Peng, X. *., A. Hunter, R. A. Lebensohn and X. Peng. Non-orthogonal computational grids for studying dislocation motion in phase field approaches. 2021. *Computational Materials Science*. **200**: 110834. (LA-UR-21-25715 DOI: 10.1016/j.commatsci.2021.110834)

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Blaschke, D., J. S. Carpenter, E. L. Tegtmeier, W. P. I. Winter, A. Hunter, C. Miller, R. M. Mier, C. M. J. Osborn, S. M. Thomas and D. R. Coughlin. Predicting electrical conductivity in Cu/Nb composites: a combined model-experiment study. . (LA-UR-22-24433)

Carpenter, J. S. Overview of Manufacturing Science Area of Leadership. Presented at *Materials Capability Review*, Los Alamos, New Mexico, United States, 2022-06-21 - 2022-06-23. (LA-CP-22-20403)

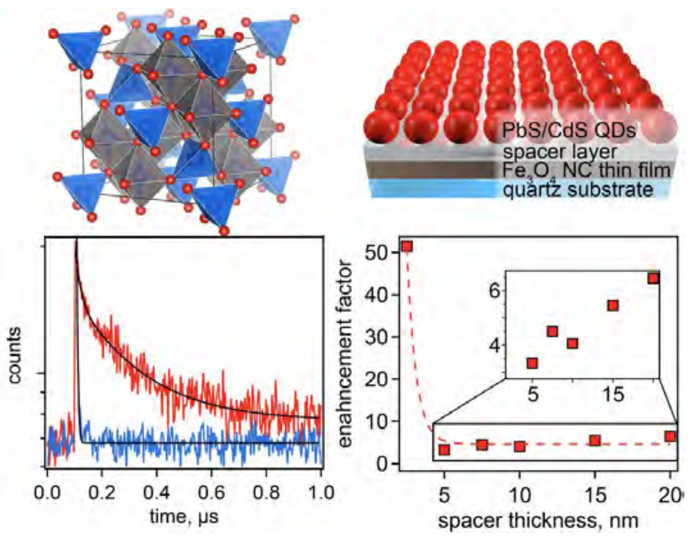
Carpenter, J. S. Overview of Manufacturing Science Area of Leadership. Presented at *Materials Capability Review*, Los Alamos, New Mexico, United States, 2022-06-21 - 2022-06-23. (LA-UR-22-25392)

Nguyen, D. N., J. S. Carpenter, A. Hunter, D. Blaschke and C. Miller. Requirement and Development of Advanced Materials To Go Beyond 100 T. Presented at *Materials Research Society (MRS) Fall Meeting and Exhibit*, Boston, Massachusetts, United States, 2022-11-27 - 2022-12-03. (LA-UR-22-32399)

**Peer-reviewed*

Emergent Infrared Localized Surface Plasmon Resonances in Doped Spinel Metal Oxide Nanomaterials

Jennifer Hollingsworth
20200407ER



The goal of this research is to develop new infrared plasmonic nanomaterials that can be used to control how light and matter interact to enable an ultrafast optical (light) alternative to nanoelectronics for communication. (Top left) A view of the inverse spinel Fe3O4 unit cell: emblematic of the structures studied here. (Top right) Schematic of the type of structure used to optimize interaction between plasmonic nanocrystals and quantum dot emitters. (Bottom left) Quantum dot (QD) fluorescence decay for QDs on chalcogenide glass (red) and on the same glass overlaying an Fe3O4 nanocrystal thin film (blue). (d) (Bottom right) The achieved Purcell enhancement factor as a function of spacer thickness.

Project Description

Near-infrared light (IR) is the foundation of fiber-optics based telecommunication technologies (1300-1550 nanometer). The range of communications and information technologies impacted by IR light sources, and the resulting market for IR solid-state lighting (SSL) sources—light-emitting diodes (LEDs) and laser diodes—is expected to dramatically expand over the next 5 years. These include LEDs for proximity sensors, eye tracking and gesture recognition and lasers for optical communication, Light Detection and Ranging (LIDAR) in automotive applications and three-dimensional (3D) facial recognition. The ability to miniaturize light sources and to easily integrate with portable/wearable/fabric technologies is key. Nanosized plasmonic materials developed here, when coupled with nanosized quantum emitters, promise new solid-state miniaturized light sources for all of these applications, which will will be critical components in a range of light-enabled, global security-relevant technologies.

Technical Outcomes

The project achieved elucidation of fundamental structure-function correlations for spinel metal oxide nanocrystals (sp-MO NCs)---novel building-block plasmonic materials for enabling efficient, miniature (and portable) infrared solid-state lighting sources and next-generation single-photon sources for the quantum-enabled internet. The project also realized the first demonstration of plasmonics-enhanced telecommunications-wavelength quantum emitters using plasmonic nanocrystals, along with a new rapid modeling capability for predicting plasmonic behavior in metal oxides based on dopability and charge carrier mobility.

Publications

Journal Articles

*Dolgopolova, E. A., D. Li, S. T. Hartman, J. Watt, C. R\xc3\xados, J. Hu, R. Kukkadapu, J. Casson, R. Bose, A. V. Malko, A. V. Blake, S. Ivanov, O. Roslyak, A. Piryatinski, H. Htoon, H. Chen, G. Pilania and J. A. Hollingsworth. Strong Purcell enhancement at telecom wavelengths afforded by spinel Fe3O4 nanocrystals with size-tunable plasmonic properties. 2022. *Nanoscale Horizons*. **7** (3): 267-275. (LA-UR-21-30232 DOI: 10.1039/D1NH00497B)

Dolgopolova, E., D. Li, J. D. Watt, C. Ocampo, J. Hu, R. Kukkadapu, J. L. Casson, R. Bose, A. V. Malko, A. V. Blake, S. A. Ivanov, H. Htoon, H. Chen, G. Pilania and J. A. Hollingsworth. Spinel Fe3O4 Nanocrystals With Size-Tunable Plasmonic Properties Afford Strong Enhancement of Emission at Telecom Wavelengths. Submitted to *Journal of the American Chemical Society*. (LA-UR-20-28261)

Dolgopolova, E., D. Li, S. T. Hartman, J. D. Watt, C. Rios, J. Hu, R. K. Kukkadapu, J. L. Casson, R. Bose, A. V. Malko, A. V. Blake, S. A. Ivanov, O. Roslyak, A. Piryatinski, H. Htoon, H. Chen, G. Pilania and J. A. Hollingsworth. Strong Purcell Enhancement at Telecom Wavelengths Afforded by Spinel Fe3O4 Nanocrystals with Size-Tunable Plasmonic Properties. Submitted to *Nanoscale Horizons*. (LA-UR-22-31497)

*Hartman, S. T. and G. Pilania. Defect thermodynamics in spinel oxides leading to plasmonic behavior. 2022. *Journal of Physics and Chemistry of Solids*. **168**: 110822. (LA-UR-21-31746 DOI: 10.1016/j.jpcs.2022.110822)

Piryatinski, A. and M. Sukharev. Degenerate parametric down-conversion facilitated by exciton-plasmon polariton states in a nonlinear plasmonic cavity. 2023. *Nanotechnology*. **34** (17): 175001. (LA-UR-22-28221 DOI: 10.1088/1361-6528/acb5a8)

Presentation Slides

Dolgopolova, E. and J. A. Hollingsworth. Alternative plasmonic nanomaterials as building blocks for Purcell-enhanced emission in the infrared. Presented at *2020 Spring ACS National Meeting, COLL Virtual Technical Symposium*, Los Alamos, New Mexico, United States, 2020-03-22 - 2020-03-24. (LA-UR-20-22500)

Dolgopolova, E. and J. A. Hollingsworth. Alternative nanomaterials with size-dependent plasmonic properties for Purcell-enhanced emission in the infrared. Presented at *ACS Fall 2020 Virtual Meeting*, San Francisco, California, United States, 2020-08-16 - 2020-08-16. (LA-UR-20-26512)

Hartman, S. T. First-principles Search for Compact Optical Materials. . (LA-UR-22-24934)

Hartman, S. T., E. Dolgopolova, G. Pilania and J. A. Hollingsworth. Theory-Guided Identification and Development of Plasmonic Spinel Oxides. Presented at *American Physical Society March Meeting*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22454)

Hollingsworth, J. A. Advanced Quantum Emitters: Chemistry, Photophysics, Integration and Application. . (LA-UR-21-24265)

Hollingsworth, J. A. Quantum Dots: From Precision Synthesis to High-Tech Applications in National Security—Part 2. . (LA-UR-21-26228)

Hollingsworth, J. A. Nano-Enabled Single-Photon Sources for Quantum Applications. Presented at *nanoGe SpringMeeting*, Virtual (international), Spain, 2022-03-07 - 2022-03-11. (LA-UR-22-22234)

Hollingsworth, J. A. Nanocrystal Quantum Emitters: From the Flask to Photonic (Quantum) Devices. Presented at *Northern Arizona University Seminar, Applied Physics and Materials Science and the Center for Materials Interfaces in Research and Applications*, Flagstaff, Arizona, United States, 2022-09-22 - 2022-09-22. (LA-UR-22-31147)

Hollingsworth, J. A. and E. L. E. McNesby. Synthesizing plasmonic shell PbS/CdS/CuxS quantum dots to enhance emission rates. . (LA-UR-21-27813)

Malone, N. A., E. G. Bowes and J. A. Hollingsworth. Synthesis of PbS/CdS/Cu2-xS Core/Shell/Shell Quantum Dots. . (LA-UR-22-28349)

Pilania, G. High throughput ab-initio and molecular dynamics studies of functional materials. . (LA-UR-22-22262)

Posters

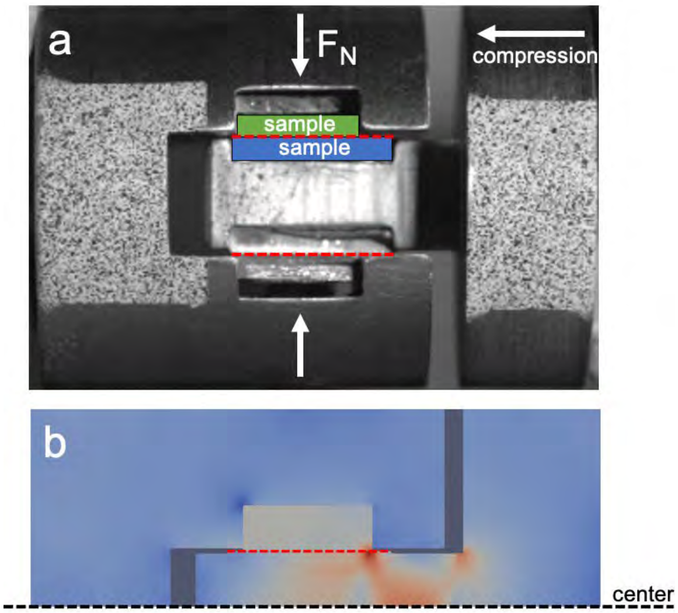
Dolgopolova, E., D. Li, J. D. Watt, G. Pilania, C. Ocampo, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Alternative Plasmonic Nanomaterials for Purcell-Enhanced Emission in the Infrared Region. Presented at *CINT Annual Meeting*, Online, New Mexico, United States, 2020-09-21 - 2020-09-24. (LA-UR-20-27165)

Nisoli, V., E. Dolgopolova, M. M. Schneider, S. T. Hartman, S. A. Ivanov, J. D. Watt, G. Pilania and J. A. Hollingsworth. Novel Spinel Metal-Oxide Nanomaterials with Infrared Plasmonic Behavior. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-07-03. (LA-UR-22-27858)

**Peer-reviewed*

Measurement of Dynamic Friction via Kolsky Bar

Benjamin Morrow
20200418ER



Dynamic friction is challenging to observe, but techniques have recently been developed to collect and analyze friction data and improve our ability to predict this important behavior. a) High-speed video is used to directly observe dynamic friction. Interfacial sliding between sets of samples (along the red dashed lines) is driven at different rates while normal force (FN) is changed to adjust friction. In tandem, the FLAG hydrocode is used to simulate friction (b), which gives a more detailed look at the microscale level. Together, these combine to allow unprecedented measuring, understanding, modeling and prediction of dynamic friction behavior.

Project Description

Friction data, especially at high rates (dynamic friction), is sparse or completely unavailable for many Laboratory-relevant materials. As a result, computational models to describe friction tend to be underdeveloped and unvalidated, decreasing confidence in simulation results. This project seeks to remedy this by 1) developing the capability to measure dynamic friction without expensive and time-consuming modifications to existing test systems, 2) validate the test technique by performing measurements at quasi-static and dynamic rates; compare with known values when possible, and generate new data where legacy testing is unavailable, and 3) mature and validate the friction models developed for a Laboratory hydrocode that is used to simulate engineering systems, improve predictive capability if necessary, and use simulations to streamline analysis of experimental tests. This program will directly contribute to filling existing gaps in experimental data, and has the potential to greatly reduce both experimental and computational uncertainties for Laboratory missions such as Stockpile Stewardship, Science Campaigns, Joint Munitions Program, and others.

Technical Outcomes

The project was successful in achieving the goals/objectives of the proposal. A capability for direct measurement of dynamic friction was developed, and a full-system model was developed for the Los Alamos National Laboratory multiphysics code FLAG to validate and develop friction submodules. New experimental capabilities are possible as a result. The project also identified several considerations for future computational work.

Publications

Journal Articles

*EUSER, V. K., D. L. WILLIAMSON, A. J. CLARKE and J. G. SPEER. Limiting Retained Austenite Decomposition in Quenched and Tempered Steels: Influences of Rapid Tempering and Silicon. 2020. *ISIJ International*. **60** (12): 2990-3000. (LA-UR-20-23093 DOI: 10.2355/isijinternational.ISIJINT-2020-263)

Euser, V. K., A. J. Clarke and J. G. Speer. Rapid Tempering: Opportunities and Challenges. Submitted to *Journal of Materials Engineering and Performance*. (LA-UR-20-24087)

Euser, V. K., D. L. Williamson, A. J. Clarke and J. G. Speer. Cementite Precipitation in Conventionally and Rapidly Tempered 4340 Steel. Submitted to *Journal of Materials*. (LA-UR-22-20168)

Euser, V. K., D. L. Williamson, K. O. Findley, A. J. Clarke and J. G. Speer. The Role of Retained Austenite in Tempered Martensite Embrittlement of 4340 and 300-M Steels Investigated through Rapid Tempering. Submitted to *Metals*. (LA-UR-21-27333)

Conference Papers

Euser, V. K., A. B. Goodbody, C. A. Yablinsky, N. A. Denissen and B. M. Morrow. Design and Simulation of Insert to Measure Dynamic Sliding Friction in a Split-Hopkinson Pressure Bar. Presented at *Dymat*. (Madrid, Spain, 2021-09-20 - 2021-09-24). (LA-UR-21-23362)

Reports

Euser, V. K., N. A. Denissen, C. A. Yablinsky and B. M. Morrow. Literature Review on the Theory and Measurement of Dry Sliding Friction of Metals. Unpublished report. (LA-UR-20-29397)

Presentation Slides

Euser, V. K., A. J. Clarke, K. O. Findley and J. G. Speer. Rapid Tempering of Quenched Martensite. Presented at *Thermec 2021*, Los Alamos, New Mexico, United States, 2021-05-11 - 2021-05-11. (LA-UR-21-21730)

Euser, V. K., B. M. Morrow, C. A. Yablinsky and N. A. Denissen. Measurement of Dynamic Friction via Kolsky Bar. . (LA-UR-21-25499)

Euser, V. K., C. A. Yablinsky, N. A. Denissen and B. M. Morrow. Co-development of Experiment and Simulation to Observe Dynamic Behavior in Metals in Complex Loading Environments. Presented at *MS&T 21*, Columbus, Ohio, United States, 2021-10-18 - 2021-10-18. (LA-UR-21-30092)

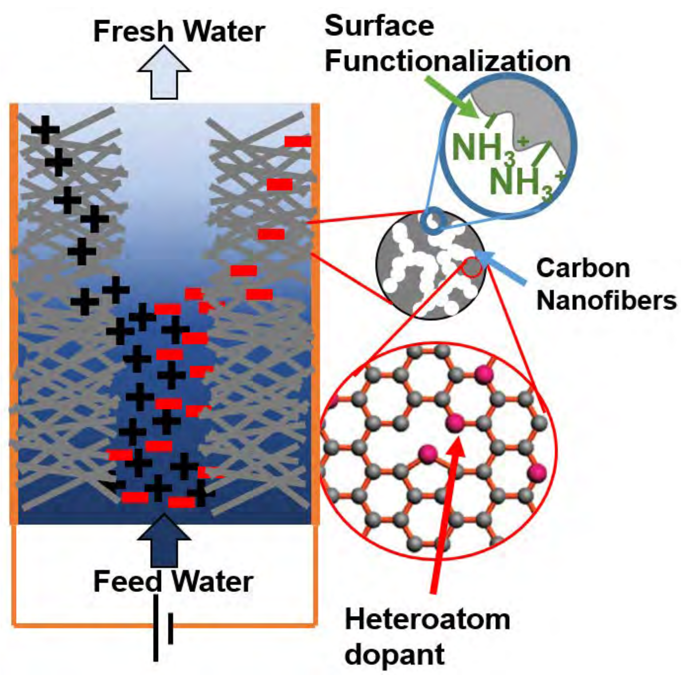
Euser, V. K., C. P. Trujillo, C. Liu, A. B. Goodbody, C. A. Yablinsky, N. A. Denissen and B. M. Morrow. Design and Simulation of Insert to Measure Dynamic Sliding Friction in a Split-Hopkinson Pressure Bar. Presented at *Dymat 2021 - 13th INTERNATIONAL CONFERENCE on MECHANICAL and PHYSICAL BEHAVIOUR of MATERIALS under DYNAMIC LOADING*, Madrid, Spain, 2021-09-20 - 2021-09-24. (LA-UR-21-29003)

Morrow, B. M., V. K. Euser, C. A. Yablinsky and N. A. Denissen. Measurement and Simulation of Dynamic Friction via Kolsky Bar Technique. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-21559)

**Peer-reviewed*

Defects and Functional Interfaces for Desalination

Jacob Spendelow
20200425ER



This project involves design of carbon nanofiber based electrodes for capacitive deionization. The team is controlling hierarchical porosity, heteroatom doping, and surface functionalization to achieve superior deionization performance.

Project Description

Access to potable water in the face of a changing climate is a key challenge facing the Department of Energy (DOE). The goal of the project is to develop cost effective desalination technology. The work involves utilizing novel structures to remove the salt from sea water effectively by adsorbing the salt on the electrode surface. The enhancements from the novel structures is projected to provide up to a 100% increase in capacity over state of the art, which could transform the desalination industry. The improved desalination technology could also enable drinking water in marine and off-shore application which are of interest to the Department of Defense (DOD).

Technical Outcomes

The project goal was to develop improved fiber-based electrodes for capacitive deionization. The team successfully fabricated electrospun carbon fiber mats with tunable morphology using heteroatom containing polymers. The resulting carbon fibers included heteroatoms such as nitrogen, increasing adsorption capacity. Electrodes with high surface area, high micro- and meso-porosity, and high ion adsorption capacity were demonstrated, and improved understanding of the effects of pore size distribution on deionization was developed.

Publications

Journal Articles

Chen, L., Q. Kang and W. Q. Tao. Pore-scale study of coupled multiphase flow and reactive transport processes in catalyst layers of proton exchange membrane fuel cells. Submitted to *International Journal of Heat and Mass Transfer*. (LA-UR-20-22352)

*Liu, M., J. Waugh, S. K. Babu, J. S. Spendelow and Q. Kang. Numerical modeling of ion transport and adsorption in porous media: A pore-scale study for capacitive deionization desalination. 2022. *Desalination*. **526**: 115520. (LA-UR-20-25564 DOI: 10.1016/j.desal.2021.115520)

Qin, F., J. Zhao, L. Fei, Q. Kang, D. Derome and J. Carmeliet. Universal scaling of nanoparticle deposition by colloidal droplet drying. Submitted to *Physical Review Letters*. (LA-UR-22-25961)

*Zhao, J., F. Qin, D. Derome, Q. Kang and J. Carmeliet. Improved pore network models to simulate single-phase flow in porous media by coupling with lattice Boltzmann method. 2020. *Advances in Water Resources*. **145**: 103738. (LA-UR-20-21321 DOI: 10.1016/j.advwatres.2020.103738)

*Zhao, J., F. Qin, Q. Kang, C. Qin, D. Derome and J. Carmeliet. A Dynamic Pore Network Model for Imbibition Simulation Considering Corner Film Flow. 2022. *Water Resources Research*. **58** (7): e2022WR032332. (LA-UR-21-32185 DOI: 10.1029/2022WR032332)

Zhao, j., F. Qin, L. Fei, C. Qin, Q. Kang, D. Derome and J. Carmeliet. Competition between main meniscus and corner film flow during imbibition in a strongly wetting square tube. 2022. *Journal of Hydrology*. **615**: 128695. (LA-UR-22-25960 DOI: 10.1016/j.jhydrol.2022.128695)

Presentation Slides

Komini Babu, S., R. Mukundan, J. S. Spendelow and A. Yilmaz. PTL Development and Characterization at LANL. Presented at *H2NEW- AMP*, Los Alamos, New Mexico, United States, 2022-03-30 - 2022-03-30. (LA-UR-22-22576)

Kang, Q. Institutional computing project annual report: Figures. . (LA-UR-22-21708)

Kang, Q. Unraveling the effects of viscous, inertial, and surface tension forces in multiphase flow using high-performance pore-scale lattice Boltzmann simulation. Presented at *M5 - Mathematics of Multiphase, Multiscale, Mutiphysics Models, Banff International Research Station for Mathematical Innovation and Discovery*, Oaxaca, Mexico, 2022-07-31 - 2022-08-05. (LA-UR-22-27938)

Kang, Q. Progress Report of Institutional Computing Project y22_CDI: Figures. . (LA-UR-23-23228)

Waugh, J. B., J. S. Spendelow and S. Komini Babu. John Waugh Qualifying Exam Presentation. Presented at *John Waugh Qualifying Exam Presentation, virtual*, Santa Fe, New Mexico, United States, 2021-08-16 - 2021-08-16. (LA-UR-21-28164)

Waugh, J. B., M. Liu, S. Komini Babu, P. Pintauro, Q. Kang and J. S. Spendelow. Generating and Optimizing Hierarchical Porosity in Electrospun Capacitive Deionization Electrodes Through Control of Mesopore Volume. Presented at *ECS 242nd Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30433)

Waugh, J. B., S. Komini Babu and J. S. Spendelow. Hierarchical Porosity in Electrospun Capacitive Deionization Electrodes. Presented at *ECS Meeting*, Atlanta, Georgia, United States, 2021-10-10 - 2021-10-14. (LA-UR-21-30487)

**Peer-reviewed*

Synchrotron-Based High-Energy Proton Radiography

Matthew Freeman
20200644ER

The facility shown here represents the next generation proton radiographic facility that we are pursuing for LANL. The data acquired here will push the envelope in terms of spatial resolution, imaging statistics, and the resolution of areal densities of materials, filling the gap in capabilities between present-day 0.8 giga-electron volt (GeV) proton radiography, and the full-scale capabilities of the Dual Axis Radiographic Hydrodynamic Test (DARHT) facility.

Project Description

We presently utilize a suite of radiographic diagnostics to probe dense, dynamic systems in pursuit of a greater understanding of their behavior. Within these capabilities, certain gaps exist, either in the available resolution, depth of material penetration, or in the available timing between image acquisitions, that leaves many questions about the expected behavior of materials unanswered. This work will evaluate a new technique that bridges some of these gaps between capabilities, by deploying proton radiography at a synchrotron facility in Germany with characteristics uniquely suited to help probe some of these unknowns. The capabilities that this would add include a factor-of-five higher proton energy that will enable the probing of denser, thicker slabs of material, as well as a x100 increase in the available protons per pulse, which will enable high fidelity imaging of very subtle effects that are presently very difficult to characterize using radiographic probes. The establishment of a collaborative effort at this early stage in the development of this new facility will pave the way towards a future collaborative effort that will yield valuable scientific results for years to come.

Technical Outcomes

The project fielded a team at the GSI accelerator facility in Darmstadt, Germany (GSI-Gesellschaft für SchwerIonenforschung- Association for Heavy Ion Research) for the 2022 proton beam run. Data was acquired with a variety of test objects using the new PRIOR-II magnifier, demonstrating high quality, 3- giga-electron volt proton data for many applications. This work was presented at the 2022 Ion Imaging Workshop in Munich and at the GSI Plasma Physics Seminar Series.

Publications

Conference Papers

R. Pelofske, E. A., A. Baertschi and S. J. Eidenbenz. Optimized Telecloning Circuits: Theory and Practice of Nine NISQ Clones. Presented at *IEEE International Conference on Rebooting Computing*. (San Francisco, California, United States, 2022-12-08 - 2022-12-08). (LA-UR-22-30899)

Reports

Freeman, M. S. PRIOR: Proton Microscope for FAIR. Shock Wave Experiements with PRIOR.. Unpublished report. (LA-UR-20-25617)

Presentation Slides

Freeman, M. S. Developments in the Development of the OMEGA Electron Radiography HED Diagnostic – Part II. Presented at *42nd International Workshop on High Energy-Density Physics with Intense Laser Beams*, Online, New Mexico, United States, 2022-02-01 - 2022-02-01. (LA-UR-22-20848)

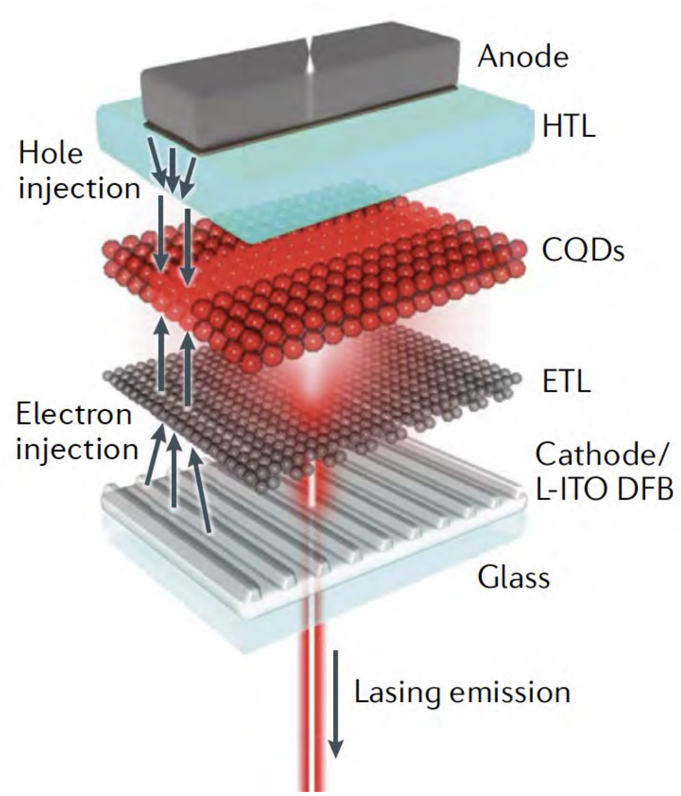
Schanz, M. 2.5-GeV proton radiography at the GSI accelerator in Darmstadt, Germany. Presented at *LANSCE User Group Meeting*, Los Alamos, New Mexico, United States, 2022-06-02 - 2022-06-03. (LA-UR-22-24959)

Schanz, M., J. C. Allison, R. Belikov, M. S. Freeman, R. Gavrilin, F. G. Mariam, D. Nikolaev, C. Morris, L. P. Neukirch, J. L. I. Schmidt, T. Schurman, A. Skobliakov and D. Varentsov. Scintillator Study Results for High Energy Particle Radiography Applications. Presented at *16th Int. Conference on Scintillating Materials & their Applications*, Santa Fe, New Mexico, United States, 2022-09-19 - 2022-09-23. (LA-UR-22-25453)

**Peer-reviewed*

Electrically Pumped Laser Processed from Solution

Victor Klimov
20210176ER



A proposed design of a laser diode based on colloidal quantum dots (CQDs) pursued in this project. It utilizes a current-focusing inverted light-emitting diode architecture that contains a second-order distributed feedback (DFB) cavity integrated into a bottom low- index indium tin oxide (L-ITO) electrode.

Project Description

This project addresses a still unresolved challenge of practically realizing an electrically pumped laser with a solution processable gain medium. The availability of such lasers would benefit numerous existing and emerging technologies including integrated electronics and photonics, optical interconnects, lab-on-a-chip platforms, wearable devices, and neuromorphic computing. Presently, several National Funding Agencies (including Department of Homeland Security, National Science Foundation, and Department of Defense) are actively pursuing new programs in areas of on-chip optical gain media and on-chip lasers as a means to enable further complexity in highly integrated electronic circuits, enhance scalability in traditional and quantum photonic circuits and push sensitivity limits in on-chip diagnostics for detecting chemical and biological hazards.

Technical Outcomes

Laser diodes based on colloidal quantum dots (QDs) are highly desired devices. However, their implementation has been hampered by ultrafast Auger recombination and poor stability of QDs at high current densities required for lasing. This project, has resolved these challenges and achieved for the first time laser action with electrically pumped QDs. The discovery paves the way for a new laser technology based on solution-processable gain media that has been pursued for decades.

Publications

Journal Articles

Ahn, N., C. Livache, V. Pinchetti, H. Jung, H. Jin, Y. Park and V. I. Klimov. Electrically Driven Laser Action Using Colloidal Quantum Dots Integrated with a Bragg-Reflector Photonic Waveguide. Submitted to *Nature*. (LA-UR-22-28400)

Ahn, N., Y. Park, C. Livache, J. Du, K. Gungor, J. H. Kim and V. I. Klimov. Optically Excited Two-Band Amplified Spontaneous Emission from a High-Current-Density Quantum-Dot LED. Submitted to *Advanced Materials*. (LA-UR-22-22960)

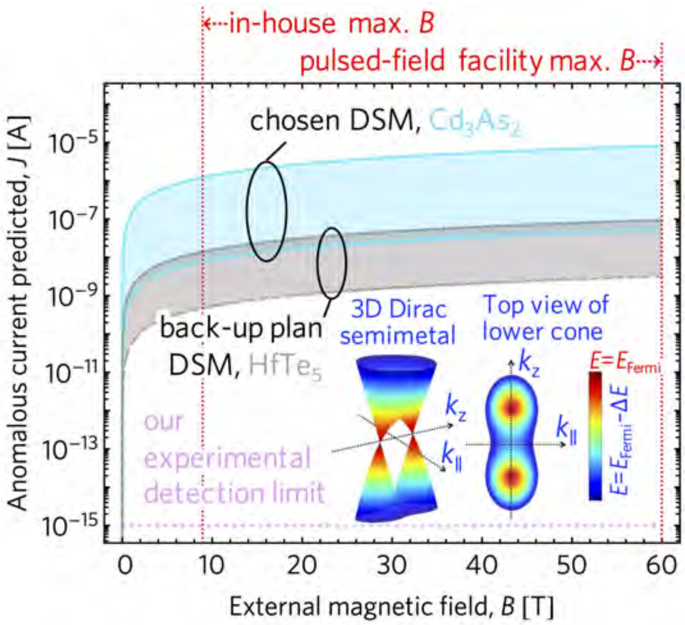
*Jung, H., N. Ahn and V. I. Klimov. Prospects and challenges of colloidal quantum dot laser diodes. 2021. *Nature Photonics*. **15** (9): 643-655. (LA-UR-21-22207 DOI: 10.1038/s41566-021-00827-6)

*Jung, H., Y. Park, N. Ahn, J. Lim, I. Fedin, C. Livache and V. I. Klimov. Two-band optical gain and ultrabright electroluminescence from colloidal quantum dots at 1000\xe2\x80\x89A\xe2\x80\x89cm−2. 2022. *Nature Communications*. **13** (1): 3734. (LA-UR-22-24389 DOI: 10.1038/s41467-022-31189-4)

**Peer-reviewed*

First Measurement of the Scale Anomaly in Dirac Semimetals

Michael Pettes
20210782ER



Predicted experimental signal of the scale anomaly supports feasibility of the approach. Predicted anomalous electric current density (J) for the Dirac Semi-Metals (DSMs) in this project. Upper and lower limits are modeled based on typical ranges for temperature gradient (0.01–0.3 K/µm), with a base temperature range of 0.75–4 Kelvin (K) for cadmium arsenide (Cd3As2) and 65 K for hafnium pentatelluride (HfTe5). (inset) Electron energy dispersion of a DSM with Dirac nodes is shown schematically.

Project Description

The scale or conformal anomaly refers to the quantum many-body effect of the dependence of coupling 'constants' upon the distance or energy scale at which they are measured. It is called a quantum anomaly because it explicitly depends upon Planck's constant, and there is no such dependence upon scale in a purely classical setting, if the Hamiltonian is scale invariant, as for example it is in the case of massless or gapless fermions. Particular interest attaches to the scale anomaly because it tracks the response of a quantum system to external gravitational fields, or in General Relativity of quantum matter to the curvature of space and time. As there are very few experimental tests of quantum theory in General Relativity, the possibility of testing the scale anomaly in a controlled laboratory environment by a relatively small and inexpensive table-top experiment is essentially unique. This project will be the only laboratory measurement – even indirectly – of the scale anomaly, and a positive measurement will have far-reaching implications for quantum effects in gravitational fields or curved spacetime, in addition to establishing a new magneto-thermal measurement capability at Los Alamos National Laboratory.

Technical Outcomes

This project's major accomplishment was growing a new material, hafnium penta-telluride, exfoliating it into a two-dimensional crystal, and transferring it onto a National High Magnetic Field Laboratory high field sample mount.

Publications

Journal Articles

Chen, L., A. X. Wu, N. Tulu, J. Wang, A. Juanson, K. Watanabe, T. Taniguchi, M. T. Pettes, M. A. Campbell, C. A. Gadre, Y. Zhou, H. Chen, P. Cao, L. A. Jauregui, R. Wu, X. Pan and J. D. Sanchez-Yamagishi. Ultrathin crystals of bismuth grown inside atomically-smooth van der Waals materials. Submitted to *Nature Nanotechnology*. (LA-UR-22-31641)

Li, X., A. C. Jones, J. Choi, H. Zhao, V. Chandrasekaran, M. T. Pettes, A. Piryatinski, N. Sinitsyn, S. A. Crooker and H. Htoon. Proximity Induced Chiral Quantum Light Generation in Strain-Engineered WSe2/NiPS3 Heterostructures. Submitted to *Nature Nanotechnology*. (LA-UR-22-20519)

*Londono-Calderon, A., R. Dhall, C. Ophus, M. Schneider, Y. Wang, E. Dervishi, H. S. Kang, C. Lee, J. Yoo and M. T. Pettes. Visualizing Grain Statistics in MOCVD WSe2 through Four-Dimensional Scanning Transmission Electron Microscopy. 2022. *Nano Letters*. **22** (6): 2578-2585. (LA-UR-21-30267 DOI: 10.1021/acs.nanolett.1c04315)

Pettes, M. T., S. Parida, Y. Wang, H. Zhao, H. Htoon, M. Chubarov, T. Choudhury, J. Redwing and A. Dongare. Tuning of the Electronic and Vibrational Properties of Epitaxial MoS2 through He-Ion Beam Modification. 2022. *Nanotechnology*. (LA-UR-22-27109 DOI: 10.1088/1361-6528/aca3af)

Wang, X., M. T. Pettes, Y. Wang, J. Zhu, R. Dhall, C. Song, A. C. Jones, J. Ciston and J. Yoo. Edge states induced enhancement of exciton-to-trion conversion in proton irradiated WS2. Submitted to *Nature Communications*. (LA-UR-22-29441)

Wang, X., R. Kaufmann, R. Chen, T. Ahmed, M. T. Pettes, P. G. Kotula, I. Bilgin, S. Kar and J. Yoo. Nucleation of Hexagonal Germanium Grains on Defect Engineered Monolayer MoS2. Submitted to *Advanced Materials*. (LA-UR-22-23843)

Zhao, H., L. Zhu, X. Li, V. Chandrasekaran, J. K. S. Baldwin, M. T. Pettes, A. Piryatinski, L. Yang and H. Htoon. Manipulating Interlayer Excitons for Ultra-pure Quantum Light Generation. Submitted to *Nature Nanotechnology*. (LA-UR-22-23118)

Presentation Slides

Campbell, M. A., S. Doan, V. Chandrasekaran, M. Dandu, A. Raja, M. T. Pettes and L. Jauregui. Towards Strain-Tuning Correlations in van der Waals Heterostructures. Presented at *EQ06.03.09: Materials Research Society (MRS) Fall Meeting and Exhibit*, Boston, Massachusetts, United States, 2022-11-27 - 2022-11-27. (LA-UR-22-32529)

Parida, S., Y. Wang, H. Zhao, H. Htoon, T. Choudhury, J. Redwing, A. Dongare and M. T. Pettes. Mechanical Tuning of the Electronic and Vibrational Properties of Epitaxial MoS2 through Ion Beam Modification. Presented at *2021 MRS Fall Meeting & Exhibit*, Boston, Massachusetts, United States, 2021-11-29 - 2021-11-29. (LA-UR-21-31636)

Pettes, M. T. Towards control over 2D material properties through ion beam modification and analysis. Presented at *CINT 2021 Annual Meeting*, Online, New Mexico, United States, 2021-09-21 - 2021-09-21. (LA-UR-21-29318)

Pettes, M. T. Emergent Phenomena in van der Waals Materials: Advancements in Characterization. Presented at *Invited talk at University of Southern California*, Los Angeles, California, United States, 2021-05-28 - 2021-05-28. (LA-UR-21-31292)

Pettes, M. T. Invited Presentation, SF15.03.01: Interface and Defect Modification of 2D Materials. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-09 - 2022-05-13. (LA-UR-22-24304)

Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials. Presented at *Invited Seminar at Texas A&M University, Department of Materials Science and Engineering*, College Station, Texas, United States, 2022-08-29 - 2022-08-29. (LA-UR-22-28999)

Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials. Presented at *Invited Seminar at University of Virginia, Department of Mechanical and Aerospace Engineering*, Charlottesville, Virginia, United States, 2022-09-15 - 2022-09-15. (LA-UR-22-29469)

Pettes, M. T. and A. B. Saxena. 20210782ER Progress FY21: First Measurement of the Scale Anomaly in Dirac Semimetals. . (LA-UR-21-30406)

**Peer-reviewed*

Self-Powered, Low Cost Semiconductors for Smart Computation

Wanyi Nie
20210783ER

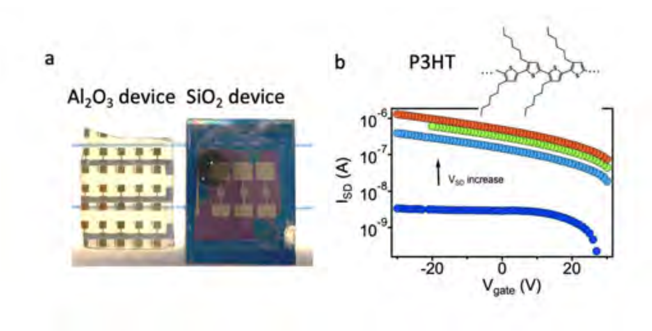


Photo and typical device characteristics being developed in this project. Here, the team will build photo-active materials on a thin film transistor. Two typical substrates are shown: a). The device's conductivity can be turned on and off by external gate voltage as shown. b). Through this project, we anticipate to deposit photo-active layer on the conducting channel, and use ambient light energy to turn the transistor on and off without low external power input.

Project Description

This project aims to explore new smart computing devices to enable artificial intelligence coupled smart electronic network. By integrating new semi conducting materials to be investigated in this project, we will develop self-powered computer element that can be operated by ambient energy. This will allow for the network to perform computation tasks without the need of external power input. The outcome from this exploratory project will open up new opportunities for smart electronics like radiation sensor, computer networks coupled with artificial intelligence. These can be used to address Department of Energy/ National Nuclear Security Administration (DOE/NNSA) missions like smart nuclear material manufacturing, remote waste treatment. It will also provide future electronic technologies to address challenges in energy and information security missions.

Technical Outcomes

The project team successfully built a theoretical coupled experimental framework to understand the defect physics of two-dimensional perovskites, and identified a few structures suitable for self-powered electronics.

Publications

Journal Articles

. G. D. *. J. K. L. *. F. D. *. S. A. *. L. S. G. *. L. F. *. N. W. *. B. J. *. Z. L. *. C. J. J. *. M. N. *. M. A. D. *. T. S. *. N. A. J. Lewis, S. G., S. G. Lewis, D. Ghosh, F. Liu, W. Nie, L. Zhou, J. J. Crochet, S. Tretiak, A. J. Neukirch and N. Moody. Cesium-Coated Halide Perovskites as a Photocathode Material: Modeling Insights. 2021. *The Journal of Physical Chemistry Letters*. **12 (27): 6269-6276. (LA-UR-21-24212 DOI: 10.1021/acs.jpclett.1c01412)

*Nie, W. and H. Tsai. Perovskite nanocrystals stabilized in metal-organic frameworks for light emission devices. 2022. *Journal of Materials Chemistry A*. **10** (37): 19518-19533. (LA-UR-22-22599 DOI: 10.1039/D2TA02154D)

*Perez, C. M., D. Ghosh, O. Prezhdo, W. Nie, S. Tretiak and A. Neukirch. Point Defects in Two-Dimensional Ruddlesden-Popper Perovskites Explored with Ab Initio Calculations. 2022. *The Journal of Physical Chemistry Letters*. **13** (23): 5213-5219. (LA-UR-22-21646 DOI: 10.1021/acs.jpclett.2c00575)

Shrestha, S., X. Li, H. Tsai, C. Hou, H. Huang, D. Ghosh, J. Shyue, L. Wang, S. Tretiak, X. Ma and W. Nie. Long carrier diffusion length in two-dimensional lead halide perovskite single crystals. Submitted to *CHEM*. (LA-UR-21-29516)

Tsai, H., D. Ghosh, E. Kinigstein, B. Dryzhakov, H. R. Driscoll, M. T. Owczarek, B. Hu, X. Zhang, S. Tretiak and W. Nie. Light Induced Structural Dynamics and the Charge Transport in Butylamine Lead Bromide Layered Perovskite Thin Films. Submitted to *Nature Materials*. (LA-UR-21-31869)

Tsai, H., D. Ghosh, E. Kinigtstein, B. Dryzhakov, H. Driscoll, M. T. Owczarek, B. Hu, X. Zhang, S. Tretiak and W. Nie. Light-Induced Structural Dynamics and Charge Transport in Layered Halide Perovskite Thin Films. 2023. *Nano Letters*. (LA-UR-22-30308 DOI: 10.1021/acs.nanolett.2c03403)

*Tsai, H., H. Huang, J. Watt, C. Hou, J. Strzalka, J. Shyue, L. Wang and W. Nie. Cesium Lead Halide Perovskite Nanocrystals Assembled in Metal-Organic Frameworks for Stable Blue Light Emitting Diodes. 2022. *Advanced Science*. **9** (14): 2105850. (LA-UR-21-30401 DOI: 10.1002/advs.202105850)

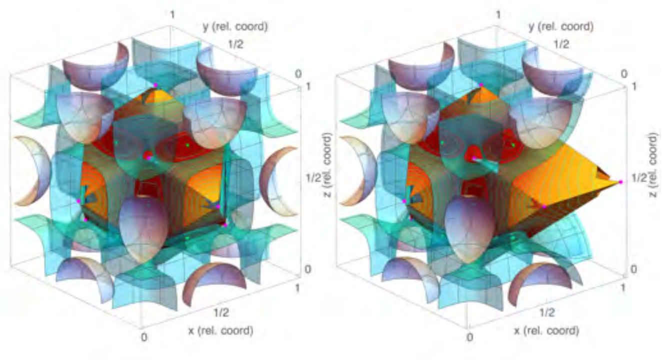
Presentation Slides

Nie, W. Low-dimensional Metal Halide Hybrid Perovskite Semiconductors for Light Emitting Devices. Presented at *Material Research Society, spring 2021*, Web meeting, New Mexico, United States, 2021-04-21 - 2021-04-27. (LA-UR-21-23773)

**Peer-reviewed*

Accurate and Local Forces for Meso-Scale Methods

Ann Wills
20210786ER



Left is a pristine aluminum lattice. Right is the same but with a vacancy on the right side. The Voronoi cells around the center ions have electron charge-density contours (cyan) on their facets, with one density surface shown in the full cells. The blue high-density spheres each have an ion in the center, and its closest point on each facet is green. The magenta points are vertices. A Voronoi cell with facets that change drastically indicates a significant rearrangement of charge, which we will use to determine a local force on the ion, replacing the expensive-to-calculate non-local force used now.

Project Description

Models of materials behavior are crucial for all computer simulations performed in science and engineering. Rubber and steel, for example, behave very differently when under pressure. At the very small scales of quantum physics (nanometers = 1 billionth of a yard) we have rigorous mathematical equations (the Dirac and Schrodinger equations) that we can solve to understand materials properties. However, at the engineering scales (millimeter = 1 million times the quantum scale), we have to infer models and parameters from macroscopic studies, mostly experiments. There is a desire to bridge this scale gap using meso-scale methods in order to improve current macro-scale materials models. But meso-scale methods currently rely on expensive-to-calculate, *non-local* forces. Based on a few fundamental theorems and conjectures, we will investigate the possibility of creating a new method for calculating *local* forces. If such a method can be developed it would revolutionize our ability to perform meso-scale simulations and considerably improve our ability to create accurate materials models for use in engineering scale codes.

Technical Outcomes

The project has shown that the information needed for calculating forces is indeed contained in the electron charge density closest to an ion. The density difference between overlapping atomic densities and the true density contains the material's bonding structure information and can be used to find an approximation for the mathematical connection between both forces and density, and density and local environment.

Publications

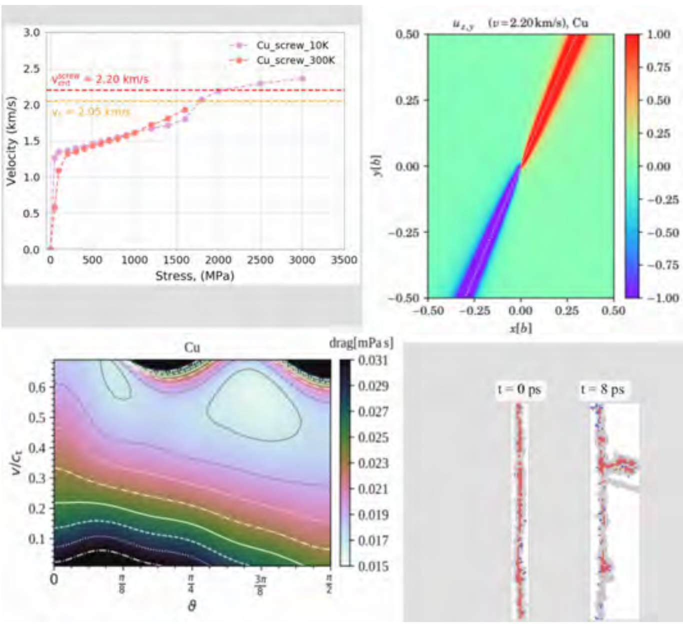
Journal Articles

Wills, A. E., S. Marrow and D. A. Rehn. Pathway to Accurate and Local Forces for Mesoscale Physics. Submitted to *Modelling and Simulation in Materials Science and Engineering*. (LA-UR-22-21704)

**Peer-reviewed*

Supersonic Dislocations? A Key to Unraveling Material Strength Under Extreme Conditions.

Daniel Blaschke
20210826ER



This project addresses the question: Under what conditions can dislocations (line defects) in metals accelerate to supersonic speeds? Answers to this question hold the key to developing a physics based predictive capability for describing plastic response of metals undergoing large, rapid deformations. The top shows the velocity of a screw dislocation versus applied stress (left) and its deformation field at high velocity (right). The bottom shows the drag coefficient (resistance to motion) of a dislocation as a function of character angle and velocity (left) and a dislocation nucleation instability in a molecular dynamics simulation (right).

Project Description

Computer simulations of materials under extreme pressure and high temperatures are needed to high precision by Los Alamos National Laboratory's national security mission. As some of these regimes cannot be directly measured, we need a good first-principles understanding of the underlying physics of dislocations (line-defects) in metals. Currently used phenomenological strength models in contrast, lack predictability beyond regimes they have been calibrated to. This is the gap we aim to fill within this project.

Technical Outcomes

This project has laid some important theoretical foundations for future improvements of strength models using first-principles. In particular, the team discovered for the first time dislocations (line defects) in an hexagonal-close-packed metal moving at supersonic speeds. Theoretical predictions of limiting velocities (separating subsonic from supersonic regimes and which are hard to overcome), were validated using molecular dynamics simulations. Finally, the influence of accelerated (in contrast to steady-state) dislocation motion on the stress field was studied.

Publications

Journal Articles

Blaschke, D., K. Q. Dang, S. J. Fensin and D. J. Luscher. Properties of accelerating edge dislocations in arbitrary slip systems with reflection symmetry. Submitted to *TBD*. (LA-UR-22-22567)

Dang, K., D. N. Blaschke, S. Fensin and D. J. Luscher. Limiting velocities and transonic dislocations in Mg. 2022. *Computational Materials Science*. **215**: 111786. (LA-UR-22-22557 DOI: 10.1016/j.commatsci.2022.111786)

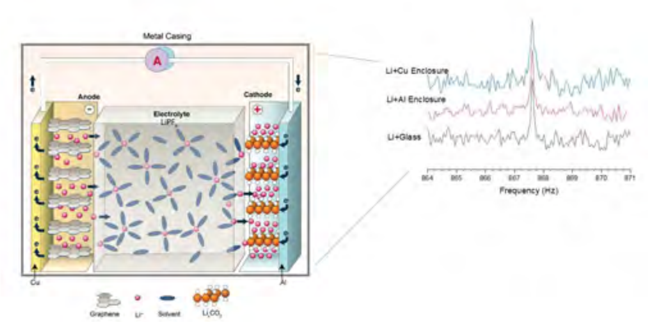
Presentation Slides

Blaschke, D., K. Q. Dang, S. J. Fensin, J. Chen, B. A. Szajewski and D. J. Luscher. Accelerating and supersonic dislocations in metals under extreme conditions. Presented at *TMS 2022 Annual Meeting & Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-21620)

**Peer-reviewed*

Using Earth's Magnetic Field for Battery Diagnostics

Benjamin Davis
20210827ER



Schematic of the battery showing the different Li components in the cathode, anode, and electrolyte. Preliminary data (right) demonstrates that the team is capable of detecting lithium (Li) through copper (Cu) and aluminum (Al) which are common to the anode and cathode in the battery. The goal of this project is to use earth's field nuclear magnetic resonance to quickly detect Li signatures of defective battery components through their metal casings to prevent these batteries from reaching consumers

Project Description

Batteries have become ubiquitous in everyday life with new applications being added every day. While battery usage is expected to drastically increase over the next 10 years, ensuring that the batteries are safe and reliable remains an outstanding issue. Many of the monitoring devices used for national security, particularly in the field, rely on these batteries and recent defects have resulted in explosions and catastrophic failure of the batteries. In this work, we will make a new type of battery diagnostic device leveraging nuclear magnetic resonance spectroscopy (NMR). This is the same technology used by medical Magnetic Resonance Imaging (MRI) instruments. In a similar manner to MRI, our device will be able to non-invasively examine the chemical composition of a sample. However, unlike MRI, which used very large magnetic fields, we propose to use Earth’s magnetic field, which is freely available through-out the world. Once the instrument is built and optimized, we will test the feasibility of detecting defects in commercially available batteries.

Technical Outcomes

The project demonstrated the ability to improve the sample transfer time from the pre-polarization magnet to the detector. The signal response for representative battery materials (Lithium Cobalt Oxide-LiCoO2), however, was not observed. By undertaking an examination of how a solution derived signal for lithium changes with increasing viscosity, the team thinks new modes of nuclear relaxation disallow a signal to be observed in solid state materials.

Publications

Journal Articles

Kaseman, D. C., P. E. Magnelind, M. T. Janicke, M. A. Alvarez, S. Widgeon Paisner, J. L. Yoder, A. Urbaitis, M. A. Espy and R. F. Williams. Advances in Earth's Field NMR for Organophosphate Chemical Warfare Agent Detection. Submitted to *Nature*. (LA-UR-22-26916)

Kaseman, D., R. J. Batrice and R. F. Williams. Detection of Natural Abundance 13C J-couplings at Earth's Magnetic Field for Spin System Differentiation of Small Organic Molecules. Submitted to *Journal of the American Chemical Society*. (LA-UR-22-22496)

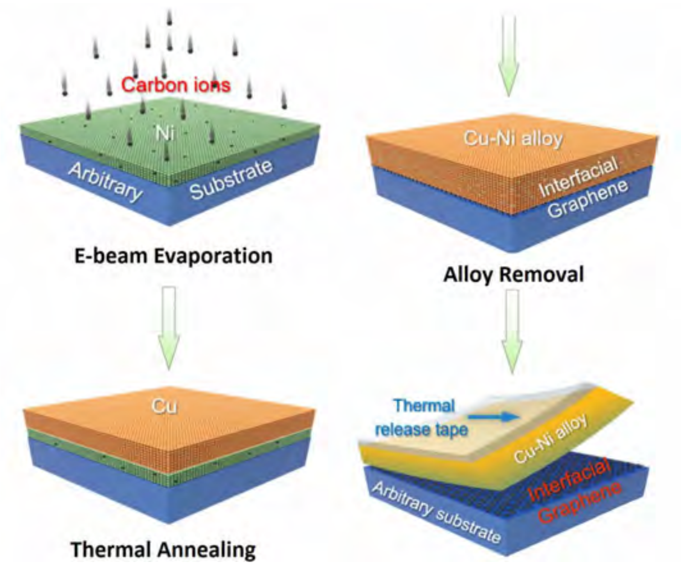
Presentation Slides

Kaseman, D. Developments in Earth's Magnetic Field NMR Spectroscopy. . (LA-UR-22-22642)

**Peer-reviewed*

Ion Beam Synthesis of Layer-Tunable, Transfer-Free and Chemically Doped Graphene Films on Arbitrary Substrates

Yongqiang Wang
20210867ER



Synthesis of layer-tunable, transfer-free, and chemically-doped graphene on arbitrary substrates remains challenging. This project aims to achieve this elusive goal through a novel ion beam synthesis approach. Our innovation is based on controlled carbon implantation and carbon-diffusion limiting process in Smart Janus Cu-Ni substrate. The layer number is precisely controlled by carbon implantation fluence. The graphene precipitation towards arbitrary substrate is facilitated by carbon solubility difference in Ni and Cu during the post-implantation annealing and CuNi alloying process. The "transfer free" step is automatically realized by removing the top CuNi alloy after the graphene is precipitated on the pre-select substrates.

Project Description

To exploit graphene as a key electronic material, with its unique two-dimensional (2D) hexagonal lattice structure and extraordinary physical properties, in nanoelectronics and flexible electronic devices applications, direct synthesis of layer-tunable graphene, independent of device substrates along with desired chemical doping characteristics, is needed. The current process involves separate growth, transfer, and doping steps. This project attempts to explore a novel ion beam-based approach that lets one synthesize doped layer-tunable graphene films on technologically-relevant substrates in a single step. The innovation is based on a large solubility difference of carbon (or boron(B)/nitrogen(N) as dopants) in different metals, e.g. a copper-nickel (Cu-Ni) bilayer smart Janus structure. During the bi-metal layer alloying process, while annealing after implantation , the pre-implanted carbon atoms (B or N dopants) are forced to precipitate onto the substrate to form a graphene film already positive- or negative-type doped due to their solubility differences between Cu and Ni. Since ion implantation is a mature technology in microelectronics industry, success of this project has potential to expedite graphene applications in versatile device applications. The materials by design knowledge gained through this project will also benefit in synthesizing other 2D quantum material structures with desired functionalities and performance characteristics.

Technical Outcomes

This project had two objectives: (1) Demonstration of layer-tunable and transfer-free graphene films on arbitrary substrates; and (2) Exploration of Layer-tunable, transfer-free and chemically doped. The team successfully achieved the first objective by demonstrating monolayer and bilayer graphene syntheses on four different substrates.

Publications

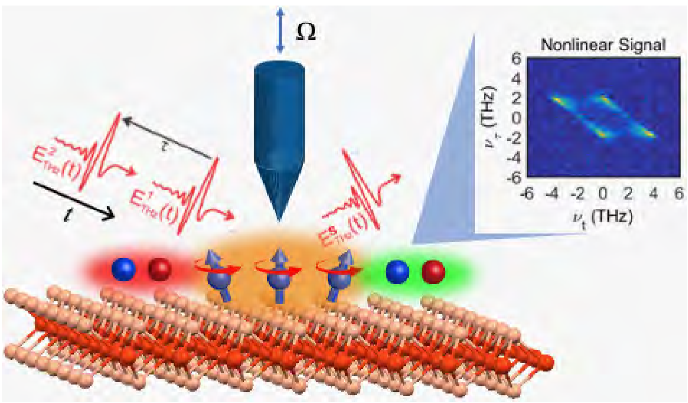
Posters

Wang, G., J. K. S. Baldwin, X. Feng, Z. Di and Y. Wang. Ion Beam Synthesis of Layer-Tunable and Transfer-Free Graphene on Arbitrary Substrates Towards Versatile Applications. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-08 - 2022-05-13. (LA-UR-22-24102)

**Peer-reviewed*

Two-Dimensional Terahertz Scanning Nanoscopy

Houtong Chen
20220661ER



(Left) Schematic showing the concept behind two-dimensional terahertz nanoscopy. (Right) Example two-dimensional spectrum, taken without spatial resolution on bismuth selenide (Bi2Se3) in the project team's labs, that will be obtained at each point on the sample.

Project Description

Characterizing excitations at low photon energies is of particular importance in quantum materials, as fundamental excitations directly associated with material properties can be selectively probed. However, significant advancement is still needed to probe and manipulate quantum states simultaneously at their ultimate length and time scales. In this project, we will establish and strengthen, in parallel, the two cornerstones of the novel technique of nonlinear two-dimensional (2D) terahertz (THz) nanoscopy: (1) THz scanning near-field optical microscopy (SNOM) and (2) 2D THz spectroscopy. The combination of these two techniques will respectively provide the required spatial and temporal resolution, thereby laying the foundation for the development of our future 2D THz nanoscopy system for studying ultrafast nanoscale quantum phenomena. The capability will provide a new window into nanoscale quantum coherence and entanglement, producing groundbreaking results that address some outstanding questions in quantum information science (QIS). Our proposed work will support and is highly relevant to Los Alamos National Laboratory's core missions in Materials for the Future. It will also establish a new capability for QIS at the Center for Integrated Nanotechnologies (CINT) as a Department of Energy national user facility.

Technical Outcomes

The team has completed the re-design of the two-dimensional terahertz spectroscopy system by observing intense terahertz pulses and allowing for the focal spot size to reduce by half at the sample as compared with the previous system, ready to characterize a number of new material systems. All components have been requisitioned, ready for setting up the terahertz scanning near-field optical microscope, marking a major milestone and sets the stage two-dimensional terahertz nanoscopy

Publications

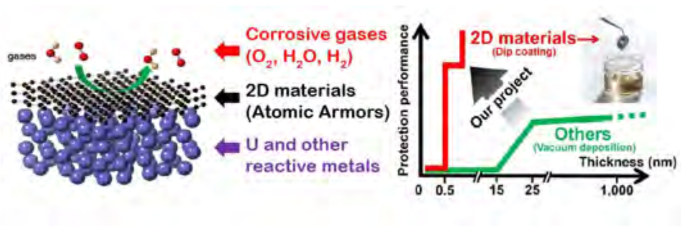
Journal Articles

Pettine, J. A., P. Padmanabhan, N. S. Sirica, R. P. Prasankumar, A. J. Taylor and H. Chen. Ultrafast Terahertz Emission from Emerging Symmetry-Broken Materials. Submitted to *Light: Science & Applications*. (LA-UR-23-20217)

**Peer-reviewed*

Two-Dimensional (2D) Materials as Corrosion Barriers for Actinides

Thomas Nizolek
20220674ER



The team will develop coatings that use 2D materials such as graphene oxide to protect mission-critical actinide metals (e.g. uranium) from corrosion, thereby extending component lifetimes (left figure). This is expected to result in a transformational improvement in the relationship between corrosion protection efficacy and coating material thickness, reducing the minimal effective coating thickness to ~1 nm from 15 nm. Additionally, these films are expected to be resistant to stress-induced cracking, a phenomenon which often severely degrades the anti-corrosion performance of thick conventional material coatings.

Project Description

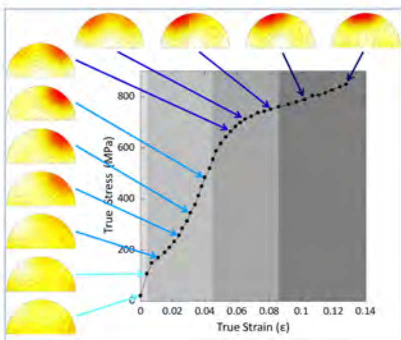
Actinide metals (e.g. uranium) are nuclear materials with tremendous importance to the Department of Energy (DOE), but these materials are highly susceptible to corrosion when exposed to common atmospheric gases. Corrosion of actinides directly impacts national security and DOE missions as it can introduce uncertainty in the service and storage lifetimes of components manufactured from these materials. Two-dimensional, atomically thin materials such as graphene oxide offer the potential to revolutionize anti-corrosion coating technology by enabling films with negligible thickness and mass to protect but not alter the physical and mechanical properties of an underlying metal component. This research will assess the potential of this emerging technology to mitigate corrosion of reactive metals, including depleted uranium, during exposure to various gas species. The development of corrosion resistant, application-appropriate, graphene oxide coatings for actinides would significantly advance the DOE missions of Nuclear Energy and Nuclear Deterrence and Stockpile Stewardship.

Technical Outcomes

This project successfully demonstrated that graphene-based two-dimensional coatings can significantly reduce the corrosion rate of highly reactive metals exposed to corrosive gas and resulted in new experimental techniques enhancing the laboratory's experimental capabilities and mission agility. Performance limiting defects in these coatings were characterized, and aspects of the coating deposition processes requiring additional development to increase the technological readiness level of this processes were identified.

Polycrystal Modeling of Uranium/Niobium(6 percent) (U – 6 wt% Nb) and Calibration Using In-Situ Neutron Diffraction Data

Donald Brown
20220696ER



The figure shows the atypical stress/strain curve of U6Nb as well as the texture evolution during deformation. Each different texture component that develops (highlight by the different backgrounds) is a signature of a distinct microscopic deformation mechanism. The current project will attempt to predict the observed properties and underlying mechanisms shown in the figure.

Project Description

There currently exists no qualified process to manufacture uranium niobium 6 percent (U6Nb) alloy components. This project will develop a microstructure aware model of the response of U6Nb to thermo-mechanical processes. That model can then be used to aid in design of future fabrication routes of specific U6Nb components and prediction of the properties of those components.

Technical Outcomes

The approach involved building upon a Los Alamos' capability/strength in the area of polycrystal plasticity modeling with models such as elastoplastic and viscoplastic self-consistent models. Preliminary work of determining the single crystal thermal expansion behavior of the monoclinic α” phase of U6Nb between 5 Kelvin (K) and 473 K was performed. This was accomplished by fitting the predictions of the polycrystalline model to in-situ diffraction measurements of the thermoelastic behavior of variously textured samples.

Publications

Presentation Slides

Agnew, S. R., D. J. Savage, N. Peterson, D. W. Brown, B. Clausen, M. Zecevic and R. A. Lebensohn. Toward an in-situ diffraction calibrated physics-based constitutive model of a shape memory alloy, U-6wt%Nb. Presented at *International Conference on Plasticity, Damage & Fracture 2023*, Punta Cana, Dominican Republic, 2023-01-03 - 2023-01-09. (LA-UR-23-20021)

**Peer-reviewed*

Kick-Starting the Hydrogen Economy with Transition Metal Nitrides

John Watt
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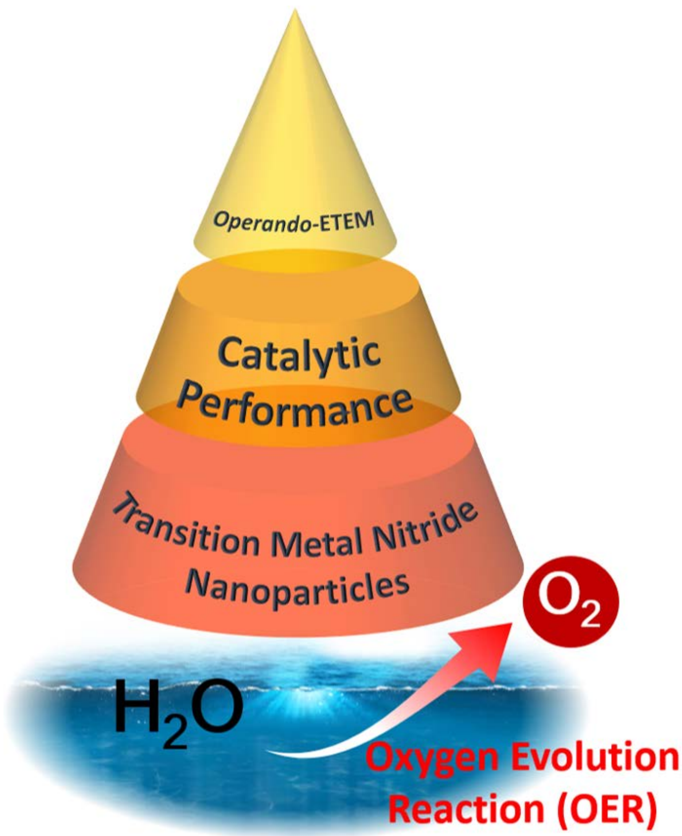


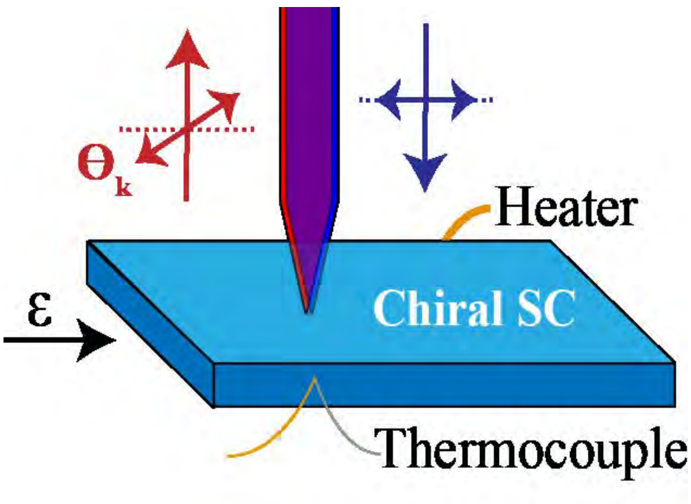
Low-cost, high-activity, stable electrocatalysts for water splitting are essential for the economical production of hydrogen as a high-density transportable fuel. The current bottleneck to achieving industrially efficiency is the sluggish oxygen evolution reaction (OER) at the anode. With LDRD support, nanoparticle synthesis, and in-situ electron microscopy we aim to produce a catalyst using earth abundant elements that displays a record low overpotential for the OER.

Project Description

Low-cost, high activity, stable electrocatalysts for water splitting are essential for the economical production of hydrogen (H2) as a high density, carbon neutral fuel. The bottleneck to achieving industrially relevant efficiency for the two component processes (hydrogen and oxygen production) is the sluggish oxygen evolution reaction (OER) at the anode. Recent studies have reported transition metal nitride (TMN) nanoparticles (NPs) with remarkably improved activity for the OER over current industry standards. However, these materials require harsh reaction conditions to form, which make it difficult to control NP composition and morphology. This lack of tight synthetic control has precluded any mechanistic understanding of their catalytic performance. A new synthetic pathway to TMN NPs must be developed, along with methods for real-time observation of structural changes during catalysis, to enable systematic analysis of fundamental structure-function relationships. This will lead to earth-abundant OER catalysts that can be actively designed to have better performance than noble metals.

Strain-Driven Demonstration of Chiral Superconductivity

Sean Thomas
20210607ECR



A chiral superconductor will cause a non-zero Kerr rotation of linearly polarized light upon reflection. Measuring Kerr rotation simultaneously with heat capacity – while applying strain to the sample – will confirm whether this exotic superconductivity exists in a number of candidate materials.

Project Description

Quantum information science is a key research area for the nation's energy and security interests. A promising route to quantum computation is to build a quantum bit using a so-called Majorana mode. A class of superconductors, called chiral superconductors, are predicted to host these Majorana modes, but unambiguous evidence of chiral superconductivity remains to be demonstrated. The goal of this project is to provide definitive proof of the chiral superconducting state through development of a new capability. This will be accomplished by combining heat capacity and uniaxial strain with a specialized optical technique.

Publications

Journal Articles

M. Girod, C. P., R. S. Callum, H. Andrew, E. D. Bauer, B. S. Frederico, J. D. Thompson, M. F. Rafael, J. Zhu, F. Ronning, P. Rosa and S. M. Thomas. Thermodynamic and electrical transport properties of UTe2 under uniaxial stress. Submitted to *Physical Review Letters*. (LA-UR-22-24502)

Presentation Slides

M. Girod, C. P., R. S. Callum, A. Huxley, E. D. Bauer, F. Santos, J. D. Thompson, R. M. Fernandes, J. Zhu, F. Ronning, P. Rosa and S. M. Thomas. Thermodynamic and electrical transport properties of UTe2 under uniaxial stress. Presented at *American Physical Society (APS) March Meeting*, las vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22251)

Thomas, S. M. Towards an understanding of the intrinsic properties in UTe2. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22285)

Posters

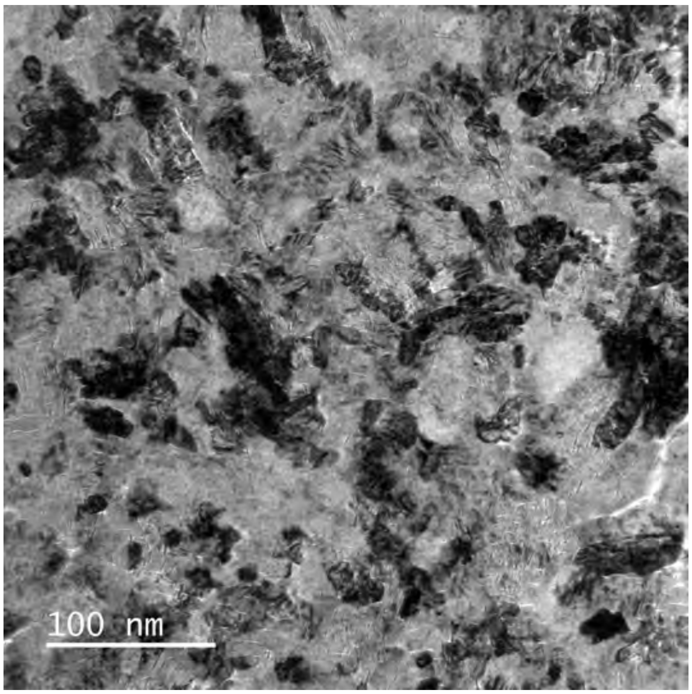
M. Girod, C. P., S. M. Thomas, P. Rosa, E. D. Bauer, J. D. Thompson, F. Ronning, J. Zhu, A. Huxley, C. Stevens, R. M. Fernandes and F. Santos. Thermodynamic and electrical transport properties of UTe2 under uniaxial stress. Presented at *29th International Conference on Low Temperature Physics*, Sapporo, Japan, 2022-08-19 - 2022-08-24. (LA-UR-22-28142)

M. Girod, C. P., S. M. Thomas, P. Rosa, F. Ronning, E. D. Bauer, J. D. Thompson, A. Huxley and C. Stevens. Mapping superconductivity with uniaxial stress in UTe2. Presented at *2022 Aspen Winter Conference, New Directions in Strong Correlation Physics: From Strange Metals to Topological Superconductivity*, Aspen, Colorado, United States, 2022-01-24 - 2022-01-28. (LA-UR-22-20243)

**Peer-reviewed*

Strong and Ductile: Towards a New Class of High Entropy Alloys with Outstanding and Optimized Properties

Osman El Atwani
20210626ECR



Transmission electron microscopy micrograph of nanocrystalline refractory W Ta Cr V based alloys achieved by LANL researchers for optimizing the ductility, strength and radiation resistance of new class of high entropy alloys.

Project Description

This project possesses interconnected experimental and modeling elements to generate a detailed understanding of chemistry and composition on the ductility of refractory four elemental alloys to optimize the performance of these alloys under extreme environments. The possible combination of elements to synthesize a four elemental alloy is virtually infinite. However, the elements are chosen to minimize radioactivity for nuclear applications. The alloys to be studied are Tungsten-Tantalum-Chromium-Vanadium (W-Ta-Cr-V) and Tungsten-Tantalum-Chromium-Iron (W Ta-Cr-Fe). These alloys will be formed in different compositions and the ductility of these alloys will be investigated. For compositions that demonstrate high ductility, other tests (such as irradiation and thermal stability) will be performed. Effect of composition on the performance of these materials will be then understood and a design of a high performance four elemental alloy will be possible.

Publications

Journal Articles

*El Atwani, O., H. Kim, C. R. Harvey, M. Efe and S. A. Maloy. Limitations of Thermal Stability Analysis via In-Situ TEM/Heating Experiments. 2021. *Nanomaterials*. **11** (10): 2541. (LA-UR-21-29330 DOI: 10.3390/nano11102541)

El Atwani, O., H. Kim, J. G. Gigax, C. R. Harvey, B. Aytuna, M. Efe and S. A. Maloy. Highly Stable, Ductile and Strong Nanocrystalline HT-9 Steels via Large Strain Machining. Submitted to *Materials & Design*. (LA-UR-21-28477)

El Atwani, O., H. T. Vo, M. A. Tunes, C. Lee, A. M. Alvarado, N. Krienke, J. Poplawsky, A. A. Kohnert, J. G. Gigax, W. Y. Chen, M. Li, Y. Wang, J. Wrobel, D. Nguyen-Manh, J. K. S. Baldwin, U. Tukac, E. Aydogan, S. J. Fensin and E. Martinez. An innovative materials design protocol for the development of novel refractory high-entropy alloys for extreme environments. Submitted to *Nature Communications*. (LA-UR-22-29831)

El Atwani, O., H. T. Vo, N. J. Krienke, E. Martinez, J. K. S. Baldwin, W. Chen, M. Li and S. J. Fensin. Are High Entropy Alloys More Radiation Resistant to loop formation than Pure Metals?. Submitted to *Materials Research Letters*. (LA-UR-22-29715)

El Atwani, O., J. G. Gigax, H. Kim, R. J. Mccabe, D. Canadinc, M. R. Chancey and J. Weaver. Micromechanical properties of spherical and facetted He bubble loaded copper. 2023. *Extreme Mechanics Letters*. 102007. (LA-UR-22-29832 DOI: 10.1016/j.eml.2023.102007)

Aydogan, E., O. El Atwani, B. Erdem, W. Chen, M. Li, A. Devaraj, B. Koc and S. A. Maloy. In-situ radiation response of additively manufactured modified Inconel 718 alloys. Submitted to *Additive Manufacturing*. (LA-UR-21-29969)

Bergstrom, Z. J., D. Perez and O. El Atwani. Helium bubble facetation in tungsten thin films. Submitted to *Scripta Materialia*. (LA-UR-22-20655)

Iroc, L., O. El Atwani, M. A. Tunes, Y. Kalay and E. Aydogan. Enhancement of the strength-ductility trade-off by transformation-induced nanolamellar structures and nanotwinning in oxygen-doped TiZrHfNbTa refractory high-entropy alloys. Submitted to *Advanced Materials*. (LA-UR-22-21273)

Picak, S., M. Vaughan, O. El Atwani, A. Mott, K. Limmer and I. Karaman. Effects of Chemical Segregation on Ductility-Anisotropy in High Strength Fe-Mn-Al-C Lightweight Austenitic Steels. 2022. *Acta Materialia*. 118589. (LA-UR-22-22745 DOI: 10.1016/j.actamat.2022.118589)

**Peer-reviewed*

Computational Modeling for the Development of Chiral Quantum Systems

Amanda Neukirch
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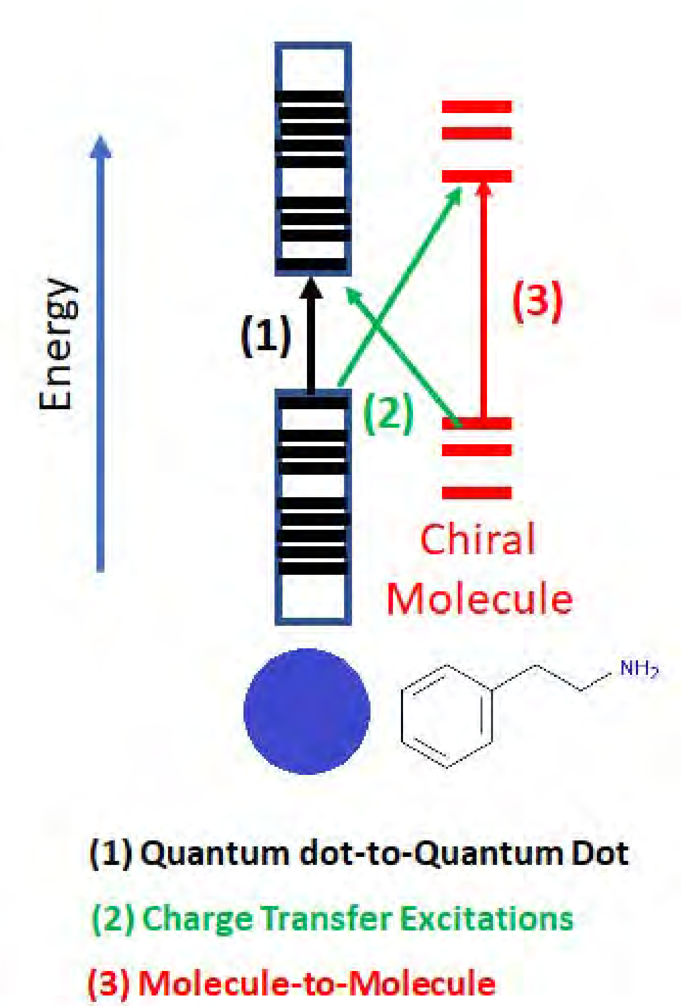


The systems being studied include a quantum dot (QD) (blue dot) with chiral molecule capping ligand. Electronic and optical transitions can take place for electronic states from the QD to the QD, between the QD to or from the chiral molecule, or from the molecule to the molecule. This project will investigate these electronic excitation and how the chirality of the system changes the electronic and optical properties.

Project Description

The term chirality is derived from the Greek word for hand and applies to any object that differs from its mirror image. All known living things are chiral. This project will study the chiroptical properties of organic ligand capped semiconductor and metallic quantum dots as they possess unique yet modular structural and optical properties not present in bulk materials. These systems are promising candidates for a broad range of applications such as drug screening, security surveillance, remote sensing, and quantum optics. Two things are needed for a direct circularly polarized light (CPL) photodetector to perform well. The first is that the absorber needs to combine handedness sensitive optical absorption (typically obtained via chiral organic ligands). The second is efficient charge transport (often best achieved with semiconductor or metallic systems). This proposal will allow for the achievement of the best of both worlds and determine structure property relationships that will allow for the controlled development of quantum chiral systems.

Publications

Journal Articles

Forde, A. A., L. A. Lystrom, W. Sun, D. S. Kilin and S. V. Kilina. Improving Near-Infrared Emission of meso-Aryldipyrrin Indium(III) Complexes via Annulation Bridging: Excited-State Dynamics. Submitted to *Chemistry of Materials*. (LA-UR-22-28183)

. G. D. *. J. K. L. *. F. D. *. S. A. *. L. S. G. *. L. F. *. N. W. *. B. J. *. Z. L. *. C. J. J. *. M. N. *. M. A. D. *. T. S. *. N. A. J. Lewis, S. G., S. G. Lewis, D. Ghosh, F. Liu, W. Nie, L. Zhou, J. J. Crochet, S. Tretiak, A. J. Neukirch and N. Moody. Cesium-Coated Halide Perovskites as a Photocathode Material: Modeling Insights. 2021. *The Journal of Physical Chemistry Letters*. **12 (27): 6269-6276. (LA-UR-21-24212 DOI: 10.1021/acs.jpclett.1c01412)

Neukirch, A. J., A. A. Forde, D. Ghosh, D. S. Kilin, A. C. Evans and S. Tretiak. Induced Chirality in Halide Perovskite Clusters through Surface Chemistry. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-29461)

*Perez, C. M., D. Ghosh, O. Prezhdo, W. Nie, S. Tretiak and A. Neukirch. Point Defects in Two-Dimensional Ruddlesden-Popper Perovskites Explored with Ab Initio Calculations. 2022. *The Journal of Physical Chemistry Letters*. **13** (23): 5213-5219. (LA-UR-22-21646 DOI: 10.1021/acs.jpclett.2c00575)

Reports

Neukirch, A. J. Computational Modeling for the Development of Chiral Quantum Systems. Unpublished report. (LA-UR-23-23333)

Neukirch, A. J., D. Ghosh, C. A. Mora Perez, O. Prezhdo, W. Nie and S. Tretiak. Impact of Compositional Engineering on Charge Carrier Cooling in Hybrid Halide Perovskites: Computational Insights. Unpublished report. (LA-UR-22-20401)

Presentation Slides

Forde, A. A. Excited state dynamics of photo-induced polarons in lead halide perovskite nanocrystals: Bright surface-trap states\xe2\x80\xaf\xc2\xa0\xc2\xa0. Presented at *The International Chemical Congress of Pacific Basin Societies (Pacifichem)*, Honalulu, Hawaii, United States, 2021-12-19 - 2021-12-19. (LA-UR-21-32290)

Forde, A. A. Induced Chirality in Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *Sanibel Symposium*, St. Simons Island, Georgia, United States, 2022-02-13 - 2022-02-18. (LA-UR-22-21246)

Forde, A. A. Induced Chirality in Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-08 - 2022-05-13. (LA-UR-22-24145)

Forde, A. A. Excited state dynamics of photo-induced polarons in lead halide perovskite nanocrystals: Bright surface-trap states\xe2\x80\xaf\xc2\xa0\xc2\xa0. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-08 - 2022-05-13. (LA-UR-22-24143)

Forde, A. A. Solvation of Molecular Excited-States: (Non)-Equilibrium Transition Energies in Donor-Acceptor. Presented at *Sanibel Symposium*, St. Augustine, Florida, United States, 2023-02-12 - 2023-02-17. (LA-UR-23-21438)

Neukirch, A. J. Nonadiabatic Dynamics Shines Light on How to Best Harness Perovskite Properties for Use in Optoelectronic Properties. Presented at *Nonequilibruim Phenomena, Nonadiabatic Dynamics and Spectroscopy*, Telluride, Colorado, United States, 2021-07-19 - 2021-07-23. (LA-UR-21-26972)

Neukirch, A. J. Harnessing the Sun and Beyond: The power of theory combined with experiment in the development of materials design for specific applications. Presented at *CINT Interview*, Los Alamos, NM, New Mexico, United States, 2022-04-27 - 2022-04-27. (LA-UR-22-23900)

Neukirch, A. J. Harnessing the Sun and Beyond: The power of theory combined with experiment in materials design for optoelectronic applications. Presented at *TSRC Workshop*, Telluride, Colorado, United States, 2022-07-12 - 2022-07-16. (LA-UR-22-26670)

Neukirch, A. J. Institutional Computing progress report: w22_chiroptical. . (LA-UR-23-23358)

Neukirch, A. J., A. A. Forde, D. Ghosh, A. C. Evans and S. Tretiak. Chirality Transfer Induced in a Lead-Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *Pacifichem 2021*, Virtual, New Mexico, United States, 2021-12-16 - 2021-12-21. (LA-UR-21-32289)

Neukirch, A. J., A. A. Forde, D. Ghosh, D. S. Kilin, A. C. Evans and S. Tretiak. Chirality Transfer Induced in a Lead-Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *APS March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22483)

Posters

Forde, A. A. Improving Near-Infrared Fluorescence Quantum Yield of meso-Aryldipyrrin Indium(III) Complexes via Annulation Bridging: A Non-Adiabatic Excited-State Dynamics Study. Presented at *Sanibel Symposium*, St. Simons Island, Georgia, United States, 2022-02-13 - 2022-02-18. (LA-UR-22-21139)

Forde, A. A., A. C. Evans, S. Tretiak and A. J. Neukirch. Towards Implementation of Modified-Redfield Theory into ab Initio Excited-State Dynamics. Presented at *Sanibel Sympsium*, St. Simons Island, Georgia, United States, 2022-02-13 - 2022-02-18. (LA-UR-22-21138)

Forde, A. A., C. A. Mora Perez, S. Tretiak and A. J. Neukirch. Physical and Chemical Modifications of Nanomaterial-

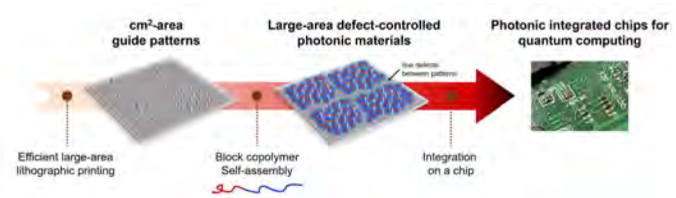
Chiral Molecule Interface for Enhanced Chirality-Transfer. Presented at *62nd Sanibel Symposium*, St. Augustine, Florida, United States, 2023-02-12 - 2023-02-17. (LA-UR-23-21201)

**Peer-reviewed*

Pattern-Assisted, Defect-Controlled Polymeric Quasicrystals for Visible-Light Integrated Photonics

Kyungtae Kim

20220525ECR



Obtaining materials with defect-controlled, self-assembled nanostructures is essential for achieving quantum optical devices that manipulate light in a new, desired way. Combining "bottom-up" mesoscale self-assembly and "top-down" lithographic printing of soft materials, researchers will develop light-propagating devices with small footprint and minimal light loss for integrated optical quantum computing applications.

Project Description

This project will provide an inexpensive, energy-efficient strategy to obtain soft-material optical devices that can process and transmit quantum information in the form of light. Light (or more generally, electromagnetic wave) is an excellent information carrier, but manipulating light propagation requires materials with precisely controlled nanostructures. By combining "top-down" lithographic printing techniques with the "bottom-up" self-assembly ability of soft materials, we will achieve macroscopic (square centimer-area) materials with controlled internal structures. This research will directly contribute to Los Alamos National Laboratory's mission-focused science, technology, and engineering by providing a new hardware technology for quantum computing, thereby asserting leadership in the national quantum initiative. In addition, the large-area nanostructure fabrication technique developed through this project will add a cutting-edge soft-material integration capability to the Lab that will potentially contribute to the Department of Engergy Basic Research Needs for Transformative Manufacturing.

Publications

Presentation Slides

LaNasa, J. A. and K. Kim. Tera Print Update. . (LA-UR-22-22534)

LaNasa, J. A. and K. Kim. Defect patterning for the directed self-assembly of block copolymers using polymer pen nanolithography. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28696)

LaNasa, J. A. and K. Kim. Soft Material Assembly Assisted with Polymer Pen Nanolithography. Presented at *Materials Research Society (MRS) Fall Meeting and Exhibit*, Boston, Massachusetts, United States, 2022-11-27 - 2022-12-02. (LA-UR-22-32437)

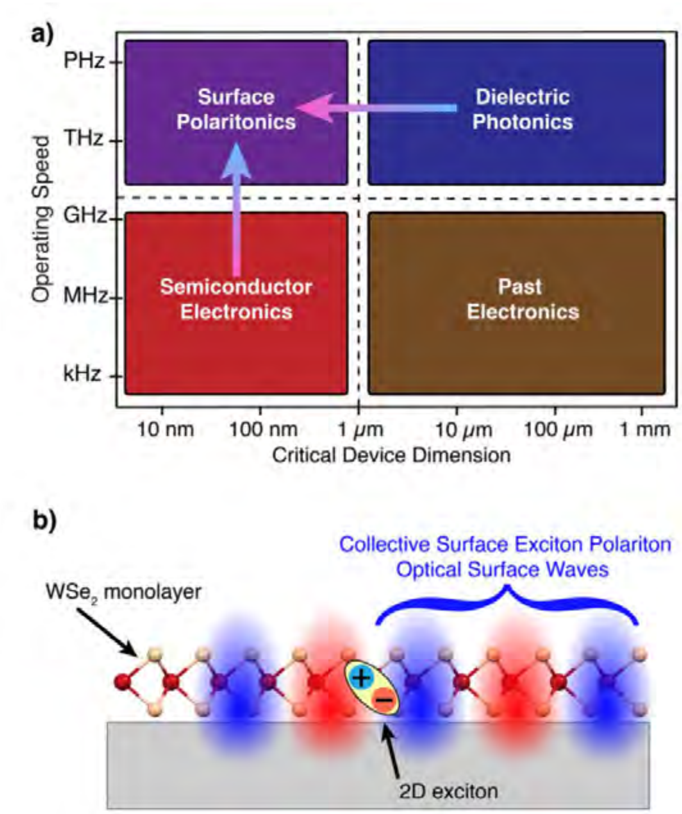
Posters

LaNasa, J. A. and K. Kim. Pattern-Assisted Assembly of Block Copolymers Using Polymer Pen Lithography for Visible-Light Photonics Applications. Presented at *Gordon Research Conference (GRC) - Polymer Physics*, South Hadley, Massachusetts, United States, 2022-07-24 - 2022-07-29. (LA-UR-22-27090)

**Peer-reviewed*

Qualification of Hybridized Exciton States as Nanoscale Information Carriers

Andrew Jones
20220531ECR



a) Semiconductor electronics are speed limited while dielectric photonics are spatially constrained by the diffraction limit. Surface Exciton Polaritons (SEPs) have the potential to bridge these regimes. b) Illustration of an SEP resulting from the hybridization of a 2D excitonic resonance with an optical surface wave.

Project Description

As improvements to classical electronic computing architectures approach their quantum limits, Moore's Law for the scaling of our computational capacity is nearing its end and we face a critical need to develop new methods of signal processing and computing. While semiconductor electronics are speed limited and dielectric photonics are spatially constrained by the diffraction limit, polaritonic carriers have the potential to bridge these regimes. The goal of this research is to identify the presence of novel electro-optical surface carriers, called surface-exciton polariton states. We seek to identify these states within target two-dimensional (2D) semiconducting materials and qualify their capability to transport classical and quantum information within nanophotonic devices. The discovery and characterization of these carriers will help form the basis for the next generation of optically based computation systems.

Publications

Journal Articles

Jones, A. C., H. Htoon, W. J. de Melo Kort-Kamp and R. A. Murdick. Leveraging eigenmode coupling in Akiyama atomic force microscopy probes for multi-frequency photoinduced force sensing. Submitted to *Nanotechnology*. (LA-UR-22-23114)

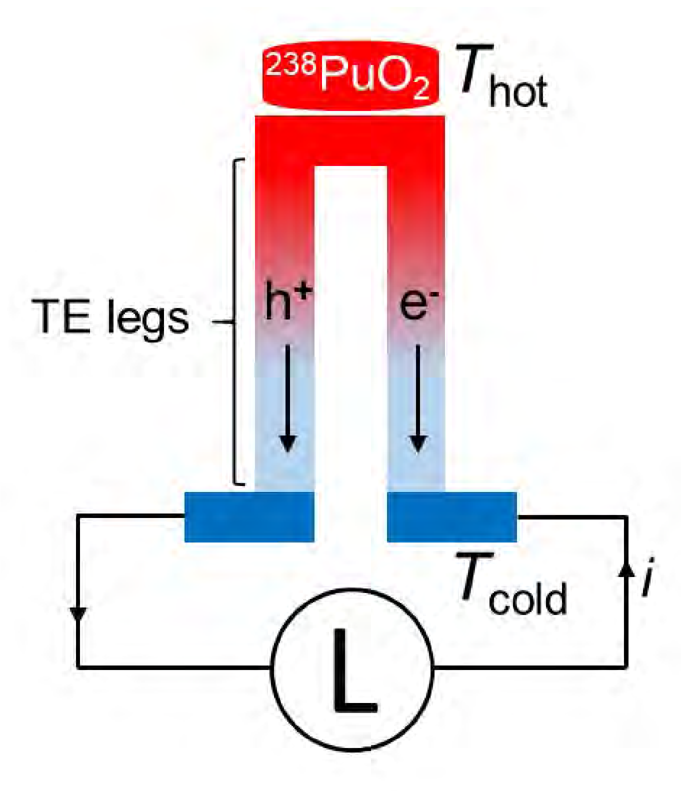
Presentation Slides

Jones, A. C., K. Kim and J. A. LaNasa. Massively parallel printing of J-aggregate dyes for the formation of optical antennas based on polariton resonances.\xc2\xa0. Presented at *Materials Research Society (MRS) Fall Meeting and Exhibit*, Boston, Massachusetts, United States, 2022-11-27 - 2022-12-02. (LA-UR-22-32376)

**Peer-reviewed*

Designing Plutonium Based Materials for Thermoelectric Optimization

William Phelan
20220538ECR



Radioisotope thermoelectric generator (RTG) schematic that can be considered the "heart" of space exploration vehicles like the Mars Perseverance Rover. Heat produced by a radioisotope near the hot side drives charges, e- and h+, in the thermoelectric (TE) legs to the generator's cold side. Usable electricity will flow if connected to a load (L). Despite plutonium's inherent properties (e.g., diffuse 5f-orbitals) having a principled promise for yielding more efficient TE legs, plutonium's contributions to RTGs have solely concerned the radioisotope. Using plutonium's properties, we will develop TE design principles that have the potential to yield RTGs that are more efficient.

Project Description

The proposed thermoelectrics (TEs), materials capable of converting waste heat into usable electricity, research directly aligns the "Actinides & Correlated Electron Materials" with the "Agile Space" investment areas described in Los Alamos National Laboratory's "Materials for the Future" strategy document. Despite TEs principled promise to deliver non-carbon based energy, their relative inefficiencies relegate their use to specialized, but relevant Department of Energy/ National Nuclear Security Administration global security applications (radioisotope TEs generators used as power sources for Mars roving vehicles). Using the inherent properties of actinides like plutonium for TEs applications remains largely unexplored, and as such, their performance will serve as a general comparative basis to current, standout non-plutonium based TEs. This in turn will help develop better, general design principles for the field of TEs, which will not only serve our countries very specialized global security needs mentioned above, but has promises to strengthen energy infrastructure (e.g., increasing power outputs of nuclear reactors, automobiles, etc.).

Predicting the Stability of Zirconium Hydride in Extreme Radiation and Thermal Environments

Caitlin Kohnert
20220597ECR

Image shows a 25 mm diameter zirconium hydride sample that fractured during fabrication by forming the hydride phase too quickly. Rapid temperature and pressure changes during operation could cause this material to fracture in a nuclear reactor. The objective of this work is to determine how radiation damage influences the behavior of zirconium hydride under different temperature conditions. Radiation effects on performance remain largely unknown.

Project Description

This work addresses the energy security challenge by improving the technological readiness of zirconium hydride for nuclear energy systems. Zirconium hydride is under consideration for use as a neutron moderator, a component that slows down neutrons to improve the efficiency of the fission chain reaction, in many nuclear energy systems. Materials in nuclear environments are exposed to high doses of radiation under extreme temperatures, but very little information exists on zirconium hydride behavior in a radiation environment. This project seeks to develop a basic understanding of zirconium hydride stability under different radiation damage doses at different temperatures, using ion irradiation as an accelerated aging technique to rapidly expose the material to specific damage doses and temperatures. Ideally, the project will result in a map of specific temperature and temperature conditions where zirconium hydride should be stable in a nuclear reactor environment. This could support component-scale neutron irradiation studies and assist engineers with selecting reactor design parameters.

Publications

Presentation Slides

Kohnert, C. A., M. A. Tunes, D. M. S. Parkison, Y. Wang, M. R. Chancey, T. Smith, A. P. Shivprasad, T. J. Nizolek, J. A. Valdez, E. P. Luther and T. A. Saleh. Phase Stability of Metal Hydrides under Combined Radiation and Thermal Environments. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-23. (LA-UR-23-22680)

Kohnert, C. A., T. J. Nizolek, A. P. Shivprasad, D. M. S. Parkison, J. R. Torres, T. Smith, M. A. Tunes, Y. Wang, M. R. Chancey, E. P. Luther and T. A. Saleh. Advanced Hydrides for Terrestrial and Space Fission Reactors. Presented at *International Conference and Expo on Advanced Ceramics and Composites*, Daytona Beach, Florida, United States, 2023-01-22 - 2022-12-27. (LA-UR-23-20066)

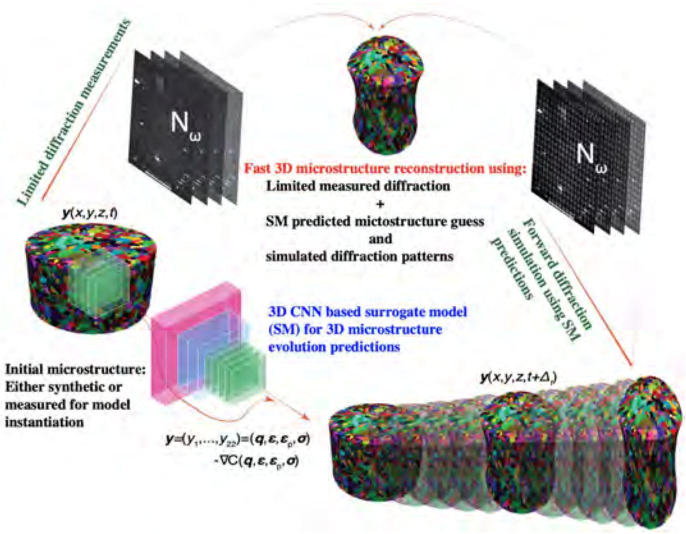
Taylor, C. A. Materials Science Capabilities in MST-8 and Sigma for Studying Metal-Hydrogen Interactions. Presented at *LANL Fusion Materials & Technology Workshop*, Los Alamos, New Mexico, United States, 2022-08-08 - 2022-08-17. (LA-UR-22-27988)

Taylor, C. A., A. P. Shivprasad, M. A. Hahn, E. L. Tegtmeier, K. R. Bohn, D. M. S. Parkison, T. J. Nizolek, R. J. Mccabe, T. Smith, M. A. Torrez, E. P. Luther and T. A. Saleh. Microstructural Comparison of Metal Hydrides Fabricated using Direct Hydriding and Powder Metallurgy Techniques. Presented at *Materials Science & Technology (MS&T) Technical Meeting*, Pittsburgh, Pennsylvania, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30350)

**Peer-reviewed*

Adaptive Framework for Enabling Real-Time Feedback During Three-dimensional Mesoscale Microstructure Evolution Measurements

Reeju Pokharel
20190571ECR



Existing materials model are unable to capture macroscopic behavior emerging from complex collective phenomena at the mesoscale. A detailed 3D view of interfaces, non-equilibrium structures, defect structures and their evolution at the mesoscale is required to develop microstructure-aware models. Although such measurements are possible at 3rd and 4th generation light sources, both data collection and reconstruction are extremely slow. The machine learning based surrogate modeling of microstructure evolution developed with LDRD support and combined with forward diffraction simulations will enable adaptive experiments by speeding up 3D microstructure measurements and reconstructions and providing real-time feedback to guide experiments at beamlines.

Project Description

This project will develop a data analysis framework that will revolutionize experiments and data analysis at current and future light sources. This project will combine state-of-the-art measurement techniques, machine learning based data analysis tools, measurement informed mechanics simulations, and adaptive model independent optimization methods to enable real-time feedback during microstructure evolution studies at light sources. The ability to provide real-time feedback during a beam line experiment will be crucial for guiding experiments that can provide information that will be crucial for influencing predictive model development. The framework will maximize the productivity and impact of a beam time and will have broad programmatic and mission impacts. Results will also be of significant interest to the light source user community and numerous collaborations will emerge as an outcome.

Technical Outcomes

This project successfully developed automatic denoising of experimental diffraction patterns and a generalized machine learning model for instantaneous microstructure reconstruction for electron backscatter diffraction. The project also developed a physics-informed surrogate model for instantaneous microstructure evolution prediction and neural-network model for instantaneous reconstruction of high-energy X-ray diffraction data. Additionally, the project developed adaptive feedback approach for improving neural-network predictions.

Publications

Journal Articles

Pandey, A., J. G. Gigax and R. Pokharel. Machine learning force-field to develop and optimize multi-components alloys. Submitted to *Computational Materials Science*. (LA-UR-22-20252)

Pandey, A. and R. Pokharel. Spatially resolved 3D microstructure evolution using long short-term memory. Submitted to *International Journal of Plasticity*. (LA-UR-20-23111)

Pandey, A. and R. Pokharel. Machine learning based surrogate modeling approach for mapping crystal deformation in three dimensions. Submitted to *Scripta Materialia*. (LA-UR-20-25246)

Pokharel, R., A. Pandey and A. Scheinker. Physics-informed data-driven surrogate modeling for full-field 3D microstructure and micro-mechanical field evolution of polycrystalline materials. Submitted to *JOM*. (LA-UR-21-25674)

Presentation Slides

R. Castillo, J. A. HEDM Reconstruction Problem. Presented at *Weekly meeting*, Los Alamos, New Mexico, United States, 2019-06-18 - 2019-06-18. (LA-UR-19-25507)

R. Castillo, J. A. Fourier Dictionary Approach for HEDM reconstruction. Presented at *weekly meeting with advisor*, Los Alamos, New Mexico, United States, 2019-07-23 - 2019-07-24. (LA-UR-19-27031)

Pandey, A. Physics-informed data-driven surrogate modeling for advancing experiments and the study of novel materials. . (LA-UR-21-27990)

Pandey, A. and R. Pokharel. Real-time analysis of diffraction data for enabling in-situ measurements. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-22416)

Pandey, A. and R. Pokharel. Physics-informed Data-driven Surrogate Modeling for Advancing Experiments and the Study of Novel Materials. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-03-03. (LA-UR-22-21816)

Pokharel, R. Data analysis framework for enabling real-time feedback during microstructure evolution. Presented at *IMS Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23306)

Pokharel, R. 3D microstructure characterization using high-energy X-rays. Presented at *3D Summer School*, Pittsburgh, Pennsylvania, United States, 2019-08-19 - 2019-08-19. (LA-UR-19-28333)

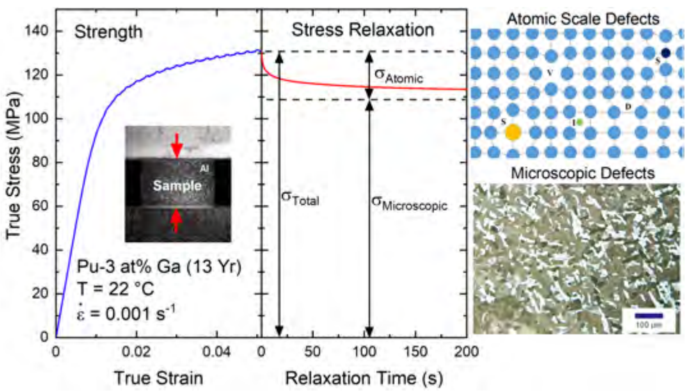
Pokharel, R. Physics-informed Data-driven Machine Learning Approach for Mesoscale Materials Science. Presented at *TMS*, Orlando, Florida, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22695)

Pokharel, R. Machine learning for real-time 3D characterization of mesoscale materials. Presented at *Engineering, Structural, and Geological Materials from Processing to Performance Workshop*, Ithaca, New York, United States, 2021-07-13 - 2021-07-13. (LA-UR-21-26437)

**Peer-reviewed*

Plutonium Defect Characterization through Mechanical Deformation

Taylor Jacobs
20200557ECR



Dislocations generated during the plastic deformation of plutonium are being used as a probe to characterize metallurgical defects associated with radioactive decay (i.e. aging). The stress relaxation technique is a mechanical test designed to separate the contributions of atomic scale and microscopic defects to the total strength of the material. When used as a complimentary technique with other characterization methods and constitutive strengthening mechanisms models, stress relaxation can help us understand illusive fundamental plutonium aging mechanisms that can impact a variety of material properties.

Project Description

Defects in a material heavily influence properties, such as strength, ductility, and toughness that are vital to engineering applications. Radiation damage occurs naturally in plutonium through radioactive decay and introduces defects over time. The characterization of defect structures in plutonium alloys during such aging is vital to the Department of Energy/National Nuclear Security Administration/Los Alamos National Laboratory strategic goal to provide a safe, secure, and effective nuclear stockpile. To this end many experimental and modeling efforts have been made to understand defect evolution during plutonium aging. Unfortunately, plutonium aging is a complex problem and a complete understanding of defect-property relationships have remained elusive. This project seeks to introduce stress relaxation and internal friction experiments to plutonium metallurgy. These mechanical testing experiments are robust, well-developed defect characterization techniques that complement the nation's existing efforts to understand aging phenomena. The team expects to see detectable changes in defect interactions in plutonium samples with different ages and processing conditions. The experimental matrix is designed to separate effects from processing and aging by working with well-characterized material from previous studies and performing a parallel set of experiments on aluminum and copper alloys that are designed to have specific defects that are relevant to plutonium.

Technical Outcomes

Stress relaxation was successfully implemented to study defects related to both aging and processing in delta phase plutonium–gallium alloys. Dislocation interactions with helium bubbles, prismatic dislocation loops, point defects, and grain boundaries were quantitatively characterized with the combination of stress relaxation experiments and a newly developed constitutive strength model that directly paralleled the stress relaxation experiments.

Publications

Journal Articles

Jacobs, T. R. Microstructure and age aware strength model for \xce\xb4-phase Pu-Ga alloys supported by stress relaxation experiments and strengthening mechanisms first principles. Submitted to *International Journal of Plasticity*. (LA-UR-22-23692)

Jacobs, T. R., J. N. Mitchell, N. M. Abdul-Jabbar, C. A. Yablinsky, Z. S. Levin and S. S. Hecker. The influence of heat-treatments and natural recovery on the strength and stress relaxation response of aged \xce\xb4-phase stabilized Pu-Ga alloys. Submitted to *Journal of Nuclear Materials*. (LA-UR-22-29333)

Reports

Jacobs, T. R., M. J. Gibbs, M. T. Janish, J. N. Mitchell, T. G. Holesinger, S. C. Vogel and S. D. Imhoff. Physical metallurgy of alloys in the Au-Zn-Al ternary system. Unpublished report. (LA-UR-22-29031)

Presentation Slides

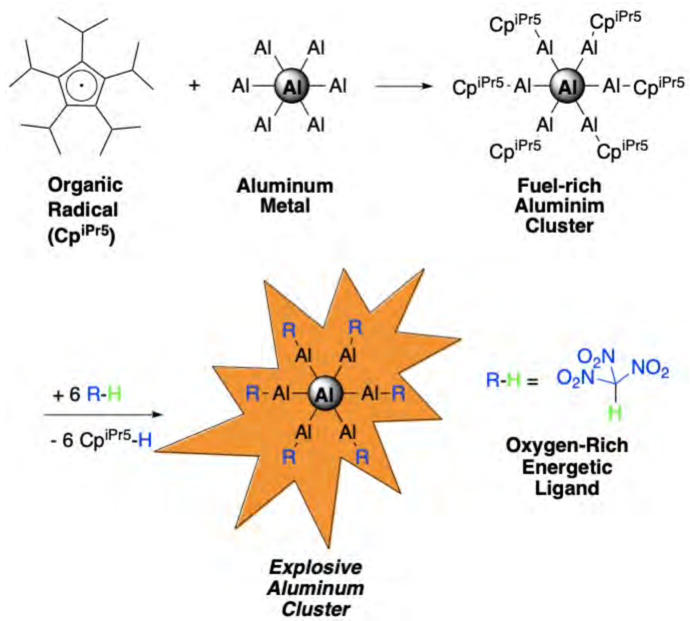
Jacobs, T. R. A Plutonium Mechanical Strength Model that Parallels Stress Relaxation Experiments. Presented at *Colorado School of Mines Invited Student Seminar Series*, Golden, Colorado, United States, 2022-03-17 - 2022-03-17. (LA-UR-22-22097)

Jacobs, T. R., M. J. Gibbs, C. A. Yablinsky, F. J. Freibert, S. C. Hernandez, J. N. Mitchell, T. A. Saleh, G. A. Kral, E. M. Solis, S. D. Imhoff, J. S. Bridgewater and D. F. Teter. Defects and Mechanical Behavior of Plutonium. . (LA-UR-20-22799)

**Peer-reviewed*

Synthesis of Aluminum Clusters as Next Generation Explosives

Christopher Snyder
20200560ECR



Aluminum is one of the most energy dense materials on Earth, however, harnessing this energy is difficult due to the presence of an aluminum oxide layer that slows down the aluminum's rate of reaction. Therefore, we are developing aluminum clusters with oxygen-rich ligands that will help facilitate fast energy release of the aluminum upon initiation. This will be achieved by first reacting aluminum with an organic radical, forming a fuel-rich aluminum cluster, which will then be reacted with an oxygen-rich energetic ligand, resulting in explosive aluminum clusters that have higher performance than conventional explosives, such as royal demolition explosive (RDX) and high melting explosive (HMX).

Project Description

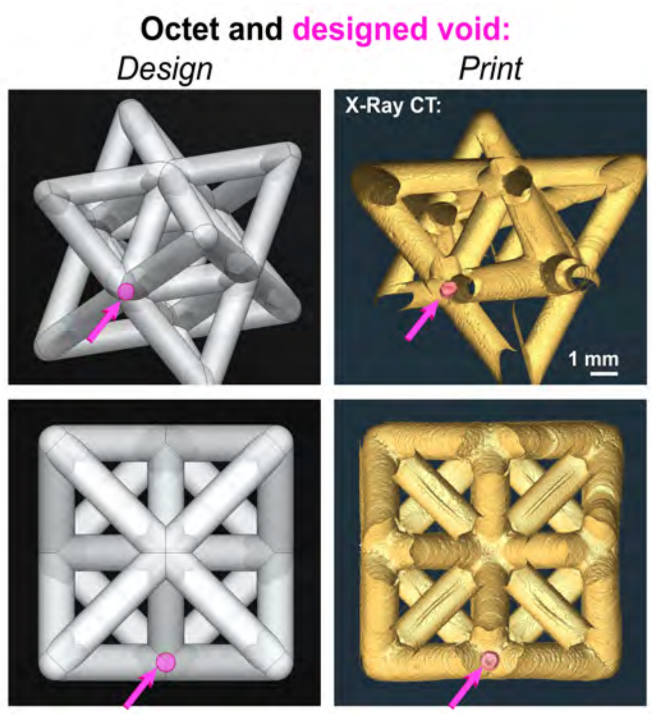
The development of new explosives with more energy than current conventional materials is important in national security. In the 156 years since the development of TNT (Trinitrotoluene), the most powerful explosive to date, CL-20 (hexanitrohexaazaisowurtzitane), is marginally better, with a detonation velocity that is only 33% higher than TNT. These materials, and most conventional explosives, are based on the elements carbon, hydrogen, nitrogen, and oxygen (CHNO). Despite the development of thousands of CHNO explosives since the discovery of TNT, obtaining an explosive with drastically better explosive properties has not been achieved. Therefore, a new approach needs to be developed to synthesize new explosives that incorporate materials that can provide better explosive performance. Aluminum-based materials have the potential to be superior to conventional explosives because aluminum has one of the highest energy densities of any material. The ultimate goal of this project is to develop aluminum clusters capped by oxygen-rich ligands as next generation explosive materials. Upon initiation, the aluminum core will react with the oxygen-rich ligands, which is predicted to release more energy than conventional explosives alone. These materials would be useful in detonators and booster applications, where there is a current need for more powerful explosive materials.

Technical Outcomes

The project has demonstrated three new concepts: The first one-electron oxidative addition to aluminum and gallium metal to form metal clusters, the first ligand exchange of the metal clusters, and the first metal clusters with oxygen-rich ligands. New bonding modes of aluminum clusters were also discovered.

The Role of Defects in Mechanical Instabilities of Additively Manufactured Lattice Materials

Rachel Collino
20200588ECR



Lattice materials are promising targets for energy absorption and light-weighting applications, but significant gaps remain in understanding processing-property-performance relationships. Additive manufacturing is typically the only route to realizing these complex geometries, but often introduces print defects that impact performance. In this project, resins and printing procedures have been developed that enable targeted and well-defined internal features (designed defects) in otherwise pristine lattice structures that enable the study of defect location and scaling on performance. This study targets the question: what are the 'killer' defect parameters critical to part screening, in-situ monitoring, and qualification?

Project Description

Three-dimensional (3D) printing has enabled the realization of geometries that were otherwise difficult or impossible to produce via traditional manufacturing techniques, including lattice materials (periodic truss structures). These structures are promising for creating lightweight materials with exceptional strength or energy absorption characteristics, but additively-manufactured lattice materials often fall short of their predicted performance. This performance gap, lack of reproducibility in mechanical behavior, and absence of a framework for part qualification all hinder the widespread adoption of lattice materials within the Department of Energy (DOE) complex. This work will use high-resolution printing techniques to create structures with intentional defect geometries, in tandem with X-Ray Computed Tomography (XCT) to observe complex structural deformations and damage evolution in 3D, to enable systematic studies of defect shape and location on failure initiation in these materials. The results will inform both simple models for screening designs (what combinations of lattice arrangement, material, and printing defects are unacceptable for a given performance criterion) as well as efforts in in-situ diagnostic development and science-based qualification.

Technical Outcomes

This project demonstrated a unique platform for realizing precise, discrete, and targeted hollow features within additively-manufactured lattice structures, allowing for the controlled study of the size, scaling, and placement of defects on the mechanical response of lattice primitives. As technologies and application evolve, this approach can be applied to more complex structures (e.g., blended lattices) and in tandem with advanced simulation (e.g., topology optimization), to provide baseline defect sensitivity studies for model calibrations.

Publications

Journal Articles

Dong, C. Q., R. R. Collino, S. P. Donegan, J. D. Miller and M. R. Begley. Effective properties for millimeter-scale struts and strut intersections (nodes) fabricated via EBM. Submitted to *TBD*. (LA-UR-21-27634)

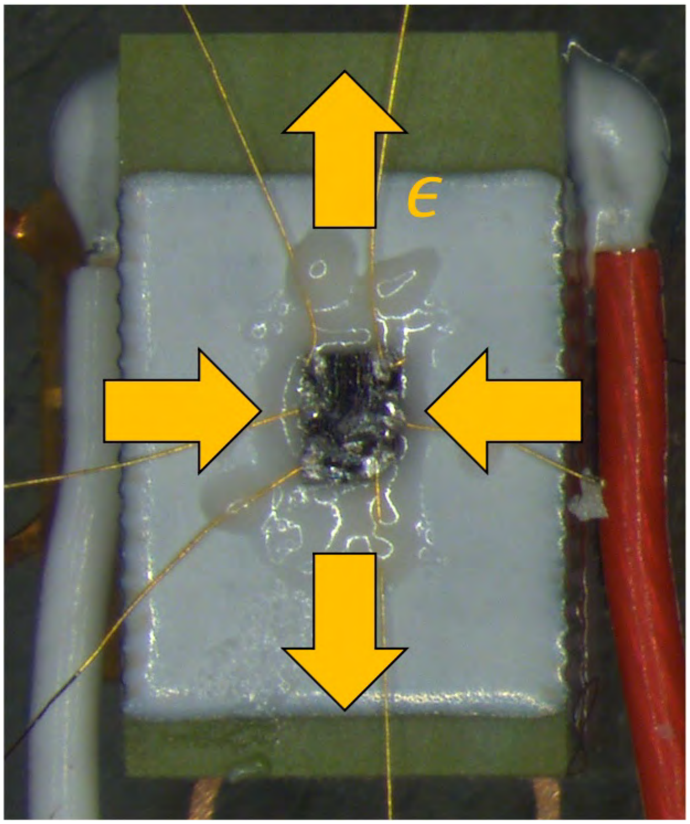
Presentation Slides

Collino, R. R., K. J. Cluff, E. A. Sandoval, R. A. (. Mikofsky, S. L. Young, L. A. Kuettner, M. N. Lee, C. J. Montgomery and B. M. Patterson. LDRD Early Career Project Update: The role of defects in mechanical instabilities of additively-manufactured lattice materials. . (LA-UR-21-27567)

**Peer-reviewed*

Strain Susceptibility of Quantum Critical Fluctuations

Johanna Palmstrom
20200680PRD1



Measurements of the electronic response to strain is one of the few symmetry sensitive measurement techniques compatible with the extreme environment of pulsed magnetic fields. Due to the coupling between electronic order and the crystal lattice, in-situ strain, depending on the symmetry, can act as either a tuning parameter for electronic phase (i.e. to suppress or enhance the transition temperature) or as a conjugate field to the electronic order (i.e. to study the strain susceptibility of the electronic fluctuations). Photograph depicts a semimetal (BaMnSb2) sample prepared for high field strain measurements.

Project Description

Electronic properties of materials can be strongly affected by applied stress. This project focuses on understanding the mechanism behind unconventional (high temperature) superconductors by measuring their electronic responses to strain in extremely high magnetic fields. There are two main goals: to develop methods of applying different symmetry strains that are compatible with pulsed magnetic field environments, and to gain a better understanding of exotic mechanisms of superconductivity. Long term, understanding superconductivity will lead to favorable material properties for quantum information processing, energy transmission and storage. Increasing the operating temperature and density of stored energy could lead to viable large-scale superconducting energy storage as an important complement to alternative energy sources. In addition, this measurement technique would be applicable to study phase transitions in a wide range of ‘mission relevant’ materials under extreme conditions. For example, actinide materials can be tuned with pressure through a variety of phase transitions, making them excellent candidate materials for strain measurements. In particular, plutonium (Pu) exhibits many structural phases and phase transitions which are not fully understood and measurements of the symmetry resolved strain susceptibility will give insights into the nature of these phase transitions.

Publications

Journal Articles

Palmstrom, J. C., P. Walmsley, J. A. W. Straquadine, M. E. Sorensen, S. T. Hannahs, D. H. Burns and I. R. Fisher. Comparison of temperature and doping dependence of elastoresistivity near a putative nematic quantum critical point. 2022. *Nature Communications*. **13** (1): 1011. (LA-UR-22-20372 DOI: 10.1038/s41467-022-28583-3)

*Pfau, H., S. D. Chen, M. Hashimoto, N. Gauthier, C. R. Rotundu, J. C. Palmstrom, I. R. Fisher, S. -. Mo, Z. -. Shen and D. Lu. Anisotropic quasiparticle coherence in nematic studied with strain-dependent ARPES. 2021. *Physical Review B*. **103** (16): 165136. (LA-UR-22-23804 DOI: 10.1103/PhysRevB.103.165136)

Reports

Palmstrom, J. C. 20200680PRD1 Data Sheet. Unpublished report. (LA-UR-21-25761)

Palmstrom, J. C. Exploring Topological Phase Transitions in Dirac Semimetals. Unpublished report. (LA-UR-22-21037)

Palmstrom, J. C. Strain Susceptibility of Quantum Critical Fluctuations. Unpublished report. (LA-UR-23-22197)

Presentation Slides

Palmstrom, J. C. Elastoresistivity of Fe-based Superconductors in High Magnetic Fields. Presented at *ARHMF2020 & KINKEN Materials Science School 2020 for Young Scientists*, Internet, Japan, 2020-12-01 - 2020-12-03. (LA-UR-20-29887)

Palmstrom, J. C. LDRD Project 20200680PRD1: Strain Susceptibility of Quantum Critical Fluctuations. Presented at *LDRD Project Visit*, Los Alamos, New Mexico, United States, 2021-05-13 - 2021-05-13. (LA-UR-21-24490)

Palmstrom, J. C. Strain as a Controllable Tuning Parameter: An in-situ Method to Break Crystal Symmetries and Change Material Properties. Presented at *Science in 3*, Los Alamos, New Mexico, United States, 2021-09-01 - 2021-09-01. (LA-UR-21-26711)

Palmstrom, J. C. High Field Elastoresistivity Measurements of Quantum Materials. Presented at *NSF site visit*, Los Alamos, New Mexico, United States, 2021-07-27 - 2021-07-27. (LA-UR-21-26712)

Palmstrom, J. C. Investigating a putative nematic quantum critical point using high magnetic field elastoresistivity measurements. Presented at *SCES 2022*, Amsterdam, Netherlands, 2022-07-24 - 2022-07-29. (LA-UR-22-27492)

Palmstrom, J. C. Strain Tuning the Room Temperature Anomalous Hall Effect in Mn3Sn. Presented at *IMS Quantum Matter Working Group*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-05. (LA-UR-22-28500)

Posters

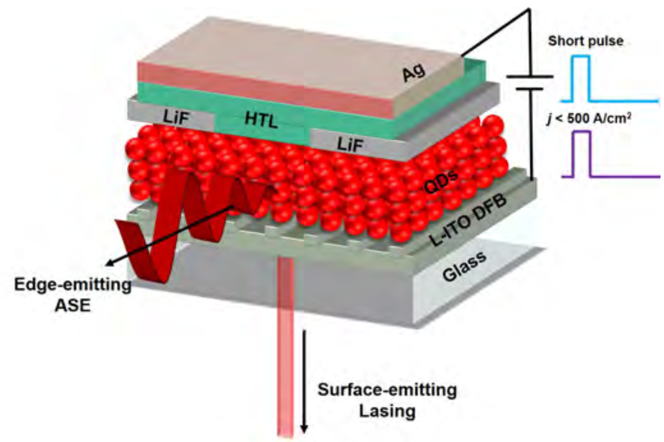
Palmstrom, J. C., N. H. Sung, P. Rosa, S. M. Thomas, E. D. Bauer, S. A. Crooker and R. D. Mcdonald. Strain tuning of the anomalous topological Hall effect at room temperature in bulk Mn3Sn. Presented at *CATS Annual Meeting 2023*, Lemont, Illinois, United States, 2023-01-12 - 2023-01-13. (LA-UR-23-20099)

Palmstrom, J. C., N. Sung, P. Rosa, S. M. Thomas, E. D. Bauer, S. A. Crooker and R. D. Mcdonald. Strain tuning of the anomalous topological Hall effect at room temperature in bulk Mn3Sn. Presented at *Gordon Research Conference (GRC & GRS) - Correlated Electron Systems*, South Hadley, Massachusetts, United States, 2022-06-25 - 2022-07-01. (LA-UR-22-25542)

**Peer-reviewed*

Electrically Pumped Laser Diodes Using Charged Colloidal Quantum Dots

Victor Klimov
20200685PRD2



A schematic depiction of a QD lasing device pursued in this project. It comprises a second-order DFB cavity integrated into a bottom L-ITO electrode, an active QD medium, and a top hole-injecting structure. The device utilizes a "current-focusing" aperture in a LiF interlayer for boosting current densities to 100s of ampere per cm2. If realized, the ultimate result of this project will be the first-ever solution-processable laser diode

Project Description

If realized, solution-processable, electrically pumped lasers (or "laser diodes") can revolutionize numerous technologies including optoelectronics, telecommunication, medical diagnostics, and homeland security. This project proposes that this challenge can be successfully tackled using specially engineered colloidal quantum dots (QDs) incorporated into "current-focusing" light emitting diodes (LED). The proposed research takes advantage of a series of recent accomplishments of Physical Chemistry Applied Spectroscopy (C-PCS) researchers that includes demonstration of QD optical gain with electrical pumping and the development of dual-function optically pumped laser/LED devices. This project's objective is to build upon these advances and demonstrate a functional QD laser diode, which will be the first practically realized solution-processable laser operating under electrical excitation. This project will apply an integrated approach: boost current density by employing a "current-focusing" LED design with short-pulse electrical pumping; enable lasing action by integrating a distributed feedback cavity into the transparent LED electrode; and enhance modal gain of a QD layer by enhancing the field confinement factor by carefully engineering a refractive-index profile across the device stack. The ultimate result of this integrated effort will be the first-ever solution-processable laser diode.

Publications

Journal Articles

Ahn, N., Y. Park, C. Livache, J. Du, K. Gungor, J. H. Kim and V. I. Klimov. Optically Excited Two-Band Amplified Spontaneous Emission from a High-Current-Density Quantum-Dot LED. Submitted to *Advanced Materials*. (LA-UR-22-22960)

Presentation Slides

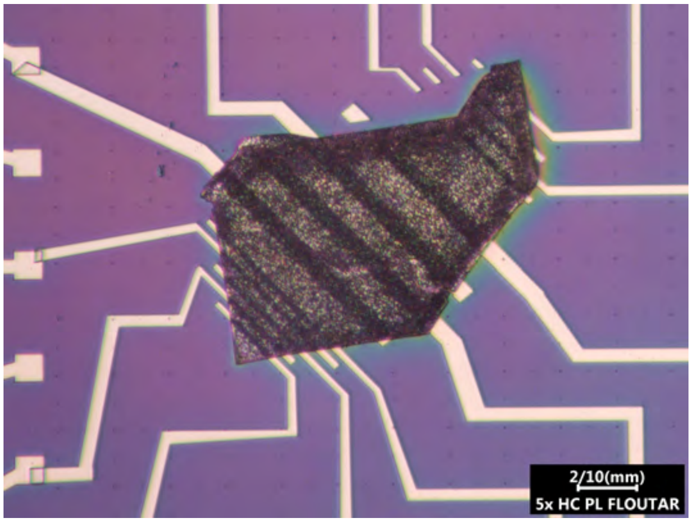
Ahn, N., Y. Park, C. Livache, J. Du and V. I. Klimov. Two-Band Optically Pumped Amplified Spontaneous Emission in an Ultrahigh-Current-Density Colloidal Quantum Dot LED. Presented at *2022 MRS spring*, honolulu, Hawaii, United States, 2022-05-08 - 2022-05-13. (LA-UR-22-24243)

Ahn, N. and V. I. Klimov. Electrically pumped laser diodes using charged quantum dots. Presented at *LDRD project visit*, Los alamos, New Mexico, United States, 2021-01-11 - 2021-01-11. (LA-UR-21-20472)

**Peer-reviewed*

Design and Discovery of Novel, Two-Dimensional Flourine-Electron Quantum Materials

Eric Bauer
20200686PRD2



Patterned device of atomically thin crystal (Ce2Te5) for investigating magnetism in the two-dimensional limit. The device will be used to measure electrical transport properties in the two-dimensional limit.

Project Description

This project will discover new two-dimensional rare earth and actinide quantum materials and investigate their novel and interesting quantum states. Quantum materials have great potential for use in future architectures for quantum computing and quantum information science to ensure the Nation's energy security.

Publications

Journal Articles

*Liu, Y., M. M. Bordelon, A. Weiland, P. F. S. Rosa, S. M. Thomas, J. D. Thompson, F. Ronning and E. D. Bauer. Physical properties of the layered f-electron van der Waals magnet Ce2Te5. 2022. *Physical Review Materials*. **6** (9): 094407. (LA-UR-22-25239 DOI: 10.1103/PhysRevMaterials.6.094407)

*Liu, Y., Z. Hu, M. Abeykoon, E. Stavitski, K. Attenkofer, E. D. Bauer and C. Petrovic. Polaronic transport and thermoelectricity in single crystals. 2021. *Physical Review B*. **103** (24): 245122. (LA-UR-21-25285 DOI: 10.1103/PhysRevB.103.245122)

*Liu, Y., Z. Hu, X. Tong, E. D. Bauer and C. Petrovic. Electrical and thermal transport in van der Waals magnets 2H-MxTaS2 (M = Mn, Co). 2022. *Physical Review Research*. **4** (1): 013048. (LA-UR-21-29465 DOI: 10.1103/PhysRevResearch.4.013048)

Mishra, S., Y. Liu, E. D. Bauer, F. Ronning and S. M. Thomas. Anisotropic magnetotransport properties of the heavy-fermion superconductor CeRh2As2. 2022. *Physical Review B*. **106** (14): L140502. (LA-UR-22-27780 DOI: 10.1103/PhysRevB.106.L140502)

Presentation Slides

Liu, Y., E. A. Ghioldi, N. Harrison, S. S. Fender, P. Rosa, J. D. Thompson, E. D. Bauer, Y. Nomura, R. Arita, Z. Wang, C. D. Batista and F. Ronning. High field magnetization anisotropy in cubic CeIn3 single crystal. Presented at *APS MArch Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22283)

**Peer-reviewed*

Highly Ordered Refractory Intermetallics: The ZIA-Phases Project

Tarik Saleh
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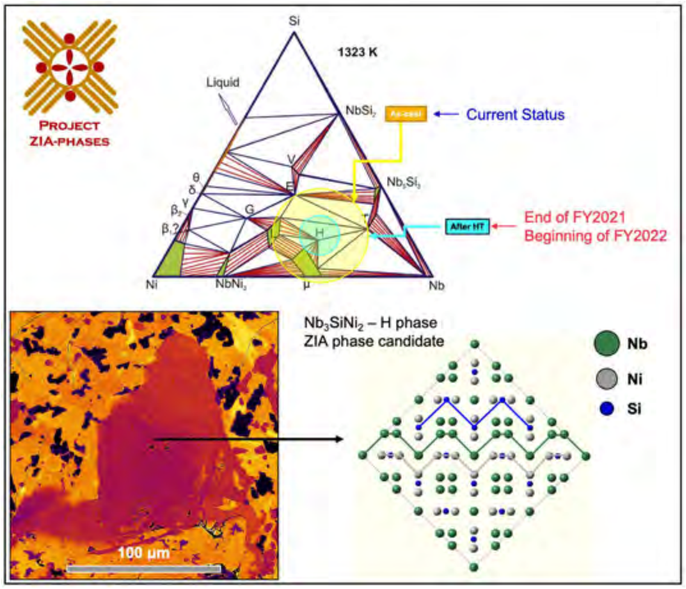


Several equilibrium phases are expected to form within the ternary system Nb-Ni-Si (niobium-nickel-silicon). The phase diagram shows the region where the first sample was synthesized (yellow circle) and the possible convergence towards the H-phase field after heat treatment. A scanning electron microscopy (SEM) micrograph shows the H-phase in the sample as cast (along with additional phases) and the projected crystalline structure, highlighting the characteristic nanolayered zig-zag.

Project Description

In this research, we propose to investigate a new class of materials, Zigzag Intermetallic Advanced Phases (ZIA) for high dose nuclear applications. We will fabricate, characterize and test these materials using high dose ion irradiation. These novel materials may have numerous nuclear reactor applications especially for use in new advanced reactors such as microreactors and Gen IV reactors such as the sodium or lead fast reactors as well as potential fusion reactor applications which have direct application to the energy security mission at Los Alamos National Lab.

Publications

Journal Articles

Coradini, D., M. A. Tunes, C. Quick, P. Willenshofer, T. Kremmer, S. Luidold, P. Uggowitzer and S. Pogatscher. Unravelling nanometallurgy with in situ electron-microscopy: a case study with Cu nanowires. Submitted to *ACS Nano*. (LA-UR-22-32828)

*Flei\xc3\x9fner-Rieger, C., M. A. Tunes, C. Gammer, T. J \xc3\xb6rg, P. Pfeifer, M. Musi, F. Mendez-Martin, H. Clemens and S. Mayer. On the existence of orthorhombic martensite in a near-\xce\xb1 titanium base alloy used for additive manufacturing. 2021. *Journal of Alloys and Compounds*. 163155. (LA-UR-21-28594 DOI: 10.1016/j.jallcom.2021.163155)

Iroc, L., O. El Atwani, M. A. Tunes, Y. Kalay and E. Aydogan. Enhancement of the strength-ductility trade-off by transformation-induced nanolamellar structures and nanotwinning in oxygen-doped TiZrHfNbTa refractory high-entropy alloys. Submitted to *Advanced Materials*. (LA-UR-22-21273)

Picak, S., P. Singh, A. Sharma, M. Lattermann, M. A. Tunes, C. R. Harvey, Y. Chumlyakov, D. D. Johnson, R. Arroyave and I. Karaman. On the origin of twinning and martensitic transformation in multi-principal element alloys. Submitted to *Science Advances*. (LA-UR-22-23701)

Picak, S., P. Singh, D. Salas, M. A. Tunes, Y. Chumlyakov, D. Johnson, R. Arroyave, Y. Ren and I. Karaman. Tailoring the Plastic Deformation in a single crystalline Medium Entropy Alloy via Short- Range Ordering. Submitted to *Nature*. (LA-UR-22-22913)

Prada-Ramirez, O., T. Kremmer, J. Marin, B. da Silva, M. Starykevich, M. A. Tunes, M. Ferreira, I. Aoki, R. Ando, S. Pogatscher and H. Melo. Ce nanoparticles and sol-gel hybrid organic-inorganic coatings maximize corrosion protection in the anodized AA2024-T3 aerospace alloy. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-23-22662)

*P. Ramirez, O. M., M. A. Tunes, M. M. Mennucci, M. Starykevich, C. Neves, M. G. S. Ferreira, S. Pogatscher and H. G. De Melo. Ce post-treatment for increased corrosion resistance of AA2024-T3 anodized in tartaric-sulfuric acid. 2022. *Corrosion Science*. **204**: 110371. (LA-UR-22-20081 DOI: 10.1016/j.corsci.2022.110371)

*Stemper, L., M. A. Tunes, R. Tosone, P. J. Uggowitzer and S. Pogatscher. On the potential of aluminum crossover alloys. 2022. *Progress in Materials Science*. **124**: 100873. (LA-UR-21-25169 DOI: 10.1016/j.pmatsci.2021.100873)

*Tunes, M. A., G. Greaves, P. Rack, W. Boldman, C. Schon, S. Pogatscher, S. A. Maloy, Y. Zhang and O. El-Atwani. Irradiation stability and induced ferromagnetism in a nanocrystalline CoCrCuFeNi highly-concentrated alloy. 2021. *Nanoscale*. **13** (48): 20437-20450. (LA-UR-21-22885 DOI: 10.1039/D1NR04915A)

Tunes, M. A., H. T. Vo, J. K. S. Baldwin, T. A. Saleh, S. J. Fensin and O. El Atwani. Perspectives on Novel Refractory Amorphous High-Entropy Alloys in Extreme Environments. Submitted to *Materials Today*. (LA-UR-22-32504)

*Tunes, M. A., M. M. Schneider, C. A. Taylor and T. A. Saleh. Rethinking radiation effects in materials science using the plasma-focused ion beam. 2022. *Journal of Materials Science*. **57** (35): 16795-16808. (LA-UR-22-26127 DOI: 10.1007/s10853-022-07667-x)

Tunes, M. A., S. Fritze, B. Osinger, P. Willenshofer, A. M. Alvarado, E. Martinez Saez, A. Menon, P. Stroem, E. Lewin, U. Jansson, S. Pogatscher, T. A. Saleh, V. Vishnyakov, O. El Atwani and G. Greaves. Nanocrystalline highly concentrated (CrNbTaTiW)C refractory high entropy ceramics with increased radiation tolerance. Submitted to *Advanced Materials*. (LA-UR-23-22313)

Tunes, M. A., S. M. Drewry, F. Schmidt, A. J. Valdez, S. J. Fensin, M. M. Schneider, C. A. Kohnert, S. A. Maloy, C. G. Sch \xc3\xb6n, O. El Atwani and T. A. Saleh. A potential class of nanolayered and chemically-complex intermetallics: the mystifying ZIA phases. Submitted to *ACS Nano*. (LA-UR-23-20139)

Tunes, M. A., S. M. Drewry, J. Arregui-Mena, S. Picak, G. Graeves, L. Cattini, S. Pogatscher, J. A. Valdez, S. J. Fensin, O. El Atwani, S. Donnelly and P. Edmondson. Accelerated radiation tolerance testing of Ti-based MAX phases. 2022. *Materials Today Energy*. 101186. (LA-UR-22-24605 DOI: 10.1016/j.mtener.2022.101186)

Willenshofer, P., M. A. Tunes, H. T. Vo, L. Stemper, O. Renk, G. Greaves, P. J. Uggowitzer and S. Pogatscher. Radiation-resistant aluminium alloy for space missions in the extreme environment of the solar system. Submitted to *Nature*. (LA-UR-22-28431)

Zhang, Y., C. Silva, T. G. Lach, M. A. Tunes, Y. Zhou, L. Nuckols, W. L. Boldman, P. D. Rack, S. E. Donnelly, L. Jiang, L. Wang and W. J. Weber. Role of Electronic Energy Loss on Defect Production and Interface Stability: Comparison between Ceramic Materials and High-Entropy Alloys. Submitted to *Current Opinion in Solid State & Materials Science*. (LA-UR-22-23704)

Presentation Slides

Arregui-Mena, J., M. A. Tunes, I. Maruyama, E. T. Rodriguez, Y. Le Pape, C. Torrence, T. M. Rosseel, T. Dixon, H. Wang and P. Edmondson. Microstructural characterization of neutron irradiated concrete aggregates. Presented at *TMS2023*, San diego, California, United States, 2023-03-20 - 2023-03-24. (LA-UR-23-22608)

Tunes, M. A. A brief history of the electronic friendship between H and Zr. Presented at *Dr. Tarik Saleh group*, Los Alamos,

New Mexico, United States, 2021-06-10 - 2021-06-10. (LA-UR-21-25482)

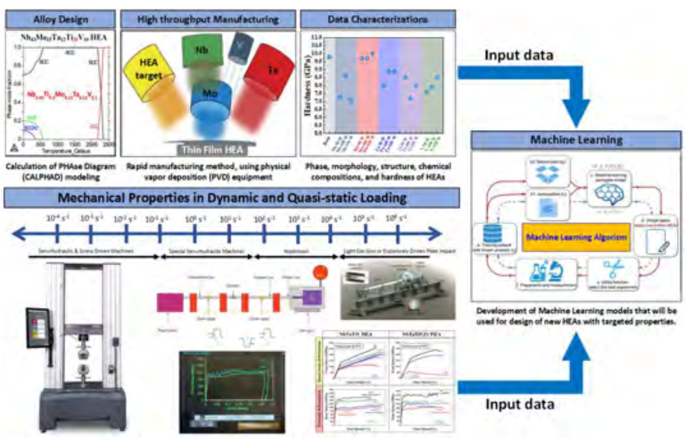
Tunes, M. A. The solar system as a new frontier for materials at extremes. . (LA-UR-22-23107)

Tunes, M. A. The solar system as a new frontier for materials at extremes. . (LA-UR-22-26678)

**Peer-reviewed*

Design and Discovery of Novel High-Entropy Alloys

Saryu Fensin
20200755PRD3



The schematic shows our overall approach to design high entropy alloys for extreme conditions. Using this approach, we have designed and manufactured 16 new compositions of high-entropy alloys (HEAs). The fabrication was performed using a high throughput approach which involves manufacturing thin films using physical vapor deposition (PVD). These films are then characterized and evaluated for their mechanical strength using various tools such as X-ray diffraction (XRD), scanning electron microscopy (SEM), electron-backscatter spectroscopy (EBSD), energy-dispersive X-ray spectroscopy (EDS) and Nano-Indenter.

Project Description

There is a need to develop materials that can withstand extreme mechanical and thermal extremes. Currently, development of many applications are limited by the availability of such materials. However, recent development of a new class of materials termed high entropy alloys provides hope as these possess a unique combination of high strength and ductility. These are metal alloys with multiple chemical elements that are combined in a specific way. Minor changes in the composition of the elements that make up these alloys can alter the material properties drastically. The combination of elements that can be used to manufacture these alloys are numerous. Hence, discovery of alloys can be time consuming. The objective of this project is to couple modeling and experiments to facilitate rapid discovery of alloys. Unlike the rest of the field using atomistic level simulations for materials discovery, the project will perform high throughput manufacturing of these materials coupled with rapid characterization that will be used to generate a database. This database will then be an input to machine learning tools. This will provide the capability to develop materials with tailored properties that will be indispensable to various projects within the National Nuclear Security Administration.

Publications

Journal Articles

*Lattice-Distortion-Enhanced Yield Strength in a Refractory High-Entropy Alloy. 2020. *Advanced Materials*. **32** (49): 2004029. (LA-UR-20-27498 DOI: 10.1002/adma.202004029)

*Investigation of phase-transformation path in TiZrHf(VNbTa)x refractory high-entropy alloys and its effect on mechanical property. 2021. *Journal of Alloys and Compounds*. **886**: 161187. (LA-UR-21-25855 DOI: 10.1016/j.jallcom.2021.161187)

*S. G. *. G. M. C. *. O. L. *. A. K. *. F. S. J. *. L. P. K. Lee, C. *., C. Lee and S. J. Fensin. Effects of Zr addition on lattice strains and electronic structures of NbTaTiV high-entropy alloy. 2022. *Materials Science and Engineering: A*. **831**: 142293. (LA-UR-22-20347 DOI: 10.1016/j.msea.2021.142293)

Lee, C., D. Xie, B. Kyle Derby, J. Kevin Baldwin, C. Tandoc, O. Ei Atwani, Y. Hu, J. A. Valdez, N. Li and S. J. Fensin. An experimentally driven high-throughput approach to design refractory high-entropy alloys. 2022. *Materials & Design*. **223**: 111259. (LA-UR-22-23502 DOI: 10.1016/j.matdes.2022.111259)

*Lee, C., F. Maresca, R. Feng, Y. Chou, T. Ungar, M. Widom, K. An, J. D. Poplawsky, Y. Chou, P. K. Liaw and W. A. Curtin. Strength can be controlled by edge dislocations in refractory high-entropy alloys. 2021. *Nature Communications*. **12** (1): 5474. (LA-UR-21-22188 DOI: 10.1038/s41467-021-25807-w)

Lee, C., J. Brechtl and P. K. Liaw. Research on Bulk-metallic Glasses and High-entropy Alloys in Peter K. Liaw's Group and with His Colleagues. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-20-30049)

*Lee, C., J. Kim, S. J. Hong, J. K. Lee, K. B. Kim, J. H. Lee, J. Han and G. Song. Development of coherent-precipitate-hardened high-entropy alloys with hierarchical NiAl/Ni2TiAl precipitates in CrMnFeCoNiAlxTiy alloys. 2021. *Materials Science and Engineering: A*. **823**: 141763. (LA-UR-21-26983 DOI: 10.1016/j.msea.2021.141763)

Presentation Slides

Lee, C., D. Xie, B. K. Derby, J. K. S. Baldwin, C. Tandoc, O. El Atwani, Y. Hu, J. A. Valdez, N. Li and S. J. Fensin. An Experimentally Driven High-throughput Approach to Design Refractory High-entropy Alloys. Presented at *Materials Science & Technology (MS&T) Technical Meeting*, Pittsburgh, Pennsylvania, United States, 2022-10-09 - 2022-10-12. (LA-UR-22-31470)

Lee, C., G. Kim, Y. Chou, B. L. Musico, M. C. Gao, K. An, G. Song, Y. Chou, V. Keppens, W. Chen and P. K. Liaw. Unique Deformation Behavior in the NbTaTiV Refractory High entropy Alloy. Presented at *TMS 2021 Annual Meeting and Exhibition*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21922)

Lee, C., G. Kim, Y. Chou, M. C. Gao, K. An, G. Song, Y. Chou, W. Chen, S. J. Fensin and P. K. Liaw. Deformation Behavior in the Refractory High-entropy Alloys. Presented at *MS&T21*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-21. (LA-UR-21-30168)

Lee, C., G. Song, M. C. Gao, W. Chen, K. An, L. Ouyang and P. K. Liaw. Distinctive Room Temperature Deformation Behavior in Plastic BCC Refractory High-entropy Alloys. Presented at *TMS 2021 Annual Meeting and Exhibition*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21902)

Lee, C., N. Li and S. J. Fensin. Design and Development of Strong and Ductile Single BCC Refractory High-entropy Alloys for Elevated-Temperature Applications. Presented at *Department Seminar at New Mexico Institute of Mining and Technology*, Socorro, New Mexico, United States, 2022-02-11 - 2022-02-11. (LA-UR-22-21042)

Lee, C., Y. Chou, G. Kim, M. C. Gao, K. An, J. Brechtl, C. Zhang, W. Chen, J. Poplawsky, G. Song, Y. Ren, Y. Chou, N. Li, S. J. Fensin and P. K. Liaw. Lattice Distortion in Refractory High-entropy Alloys. Presented at *2021 Virtual MRS Spring Meeting & Exhibit*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-23. (LA-UR-21-23819)

**Peer-reviewed*

Characterizing the Spatial and Temporal Evolution of Nuclear Materials during Coupled Irradiation and Corrosion

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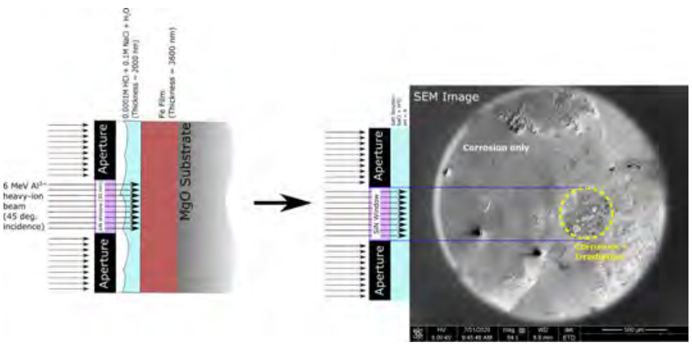
20210760PRD1



Materials used in nuclear-reactor environments are exposed to corrosion and irradiation simultaneously. We do not currently understand the physical mechanisms that control corrosion of a material being exposed to simultaneous irradiation. This image represents the novel in situ characterization cell the project team has designed with LDRD support to fit inside a scanning electron microscope such that we can image a material surface as it is being exposed to irradiation and corrosion. This capability will allow the team to more fully understand how irradiation enhances or retards the corrosion process to help inform nuclear-material choice and design.

Project Description

The goal of this project is to develop a novel in situ testing devices to study materials response at a coupled corrosion and irradiation extremes. This proposal seeks to identify the underlying principles that control material expression in extreme environments by conducting in situ (i.e. with irradiation at the same time) diagnostic testing on corrosion mechanisms in nuclear-relevant materials. Outstanding scientific questions in this field include how complex oxides grow in extreme environments and how irradiation effects the overall corrosion behavior of materials. To solve these questions and, more importantly, to inform the design of materials that better withstand degradation in this environment of coupled extremes, in situ characterization of the temporal and spatial development of complex oxides on metallic materials is needed.

Publications

Journal Articles

Derby, B. K., Y. Sharma, J. A. Valdez, M. R. Chancey, Y. Wang, E. L. Brosha, D. J. Williams, M. M. Schneider, A. Chen, B. P. Uberuaga, C. Kreller and M. T. Janish. Interfacial cation mixing and microstructural changes in bilayer GTO/GZO thin films after irradiation. Submitted to *Journal of Materials*. (LA-UR-22-21386)

Lang, E., N. Heckman, T. Clark, B. K. Derby, A. Barrios, A. Monterrosa, B. Muntifferinga, C. Barr, D. Buller, D. Stauffer, N. Li, B. L. Boyce, S. Briggs and K. Hattar. Development of an In situ Ion Irradiation Scanning Electron Microscope. Submitted to *NIMB*. (LA-UR-22-28737)

*Paudel, B., Y. Sharma, B. K. Derby, G. Pilania, M. M. Schneider, A. C. Jones, H. Nakotte, M. T. Pettes and A. Chen. Effect of lattice strain on magnetism in epitaxial YCrO3 films. 2022. *Materials Research Letters*. **10** (1): 29-35. (LA-UR-21-30206 DOI: 10.1080/21663831.2021.2010822)

*Powers, M., B. Derby, S. N. Manjunath and A. Misra. Hierarchical morphologies in co-sputter deposited thin films. 2020. *Physical Review Materials*. **4** (12): 123801. (LA-UR-22-24766 DOI: 10.1103/PhysRevMaterials.4.123801)

Sahu, B., W. Higgins, B. K. Derby, G. Pharr and A. Misra. Strain-rate dependent deformation mechanisms in single-layered Cu, Mo, and multilayer Cu/Mo thin films. Submitted to *Materials Science & Engineering A: Structural Materials: Properties, Microstructures and Processing*. (LA-UR-22-30584)

*Terricabras, A. J., L. Wang, A. M. Raftery, A. T. Nelson and S. J. Zinkle. Properties and microstructure evolution of silicon nitride and zirconium nitride following Ni ion irradiation. 2022. *Journal of Nuclear Materials*. **563**: 153643. (LA-UR-21-31255 DOI: 10.1016/j.jnucmat.2022.153643)

Presentation Slides

Derby, B. K., C. Kreller and M. T. Janish. Interfacial cation mixing and microstructural changes in bilayer GTO/GZO thin films after irradiation. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-28 - 2022-03-03. (LA-UR-22-21547)

Derby, B. K., E. Lang, T. Clark, K. Hattar, J. Han, C. Kreller, M. T. Janish and N. Li. Characterizing the Spatial and Temporal Evolution of Iron Thin Films During Coupled Irradiation and Corrosion. Presented at *MS&T 2021*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-17. (LA-UR-21-29912)

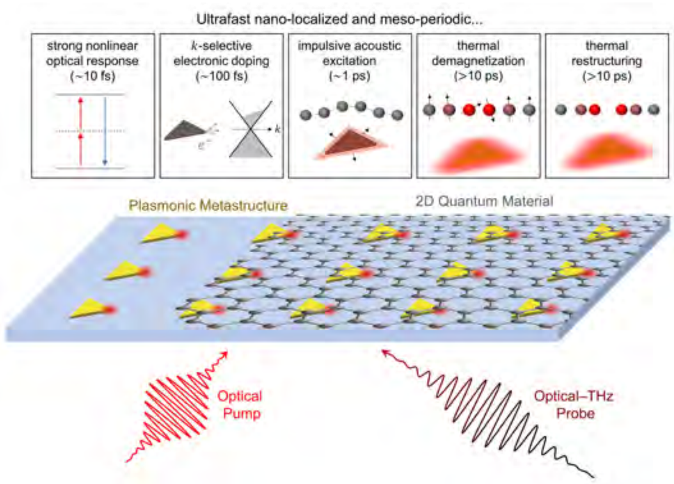
Posters

Derby, B. K., Y. Sharma, J. A. Valdez, M. R. Chancey, Y. Wang, E. L. Brosha, D. J. Williams, M. M. Schneider, A. Chen, B. P. Uberuaga, C. Kreller and M. T. Janish. Cation Mixing and Microstructural Changes at Complex Oxide Interfaces After Irradiation. . (LA-UR-22-29448)

**Peer-reviewed*

Ultrafast Spectroscopy of Hybrid Quantum-Plasmonic Nanoscale Optical Systems

Houtong Chen
20210845PRD1



Schematic showing the ultrafast processes that occur after optical excitation in a two-dimensional quantum material combined with a plasmonic metastructure. By characterizing these responses, light-matter interactions can be significantly enhanced for applications in quantum information science (QIS) and scalable optical circuits.

Project Description

The goal of this project is to combine plasmonic structures, which control directional light flow at the nanoscale, with atomically thin two-dimensional quantum materials, which can provide new materials functionality, allowing us to enhance light-matter interactions with these hybrid nanostructures for a host of potential applications. This directly impacts national initiatives in quantum information science, which will underpin a host of future applications (e.g., quantum computing, secure communications, etc.). It will also address Department of Energy (DOE)/National Nuclear Security Administration (NNSA) priorities in next generation quantum systems, quantum materials, and ultrafast science. Finally, we anticipate potential connections to several DOE/NNSA missions, including the development of new materials and approaches for global security as well as novel approaches to quantum transduction that could impact optical communications.

Publications

Journal Articles

Pettine, J. A., P. Padmanabhan, N. S. Sirica, R. P. Prasankumar, A. J. Taylor and H. Chen. Ultrafast Terahertz Emission from Emerging Symmetry-Broken Materials. Submitted to *Light: Science & Applications*. (LA-UR-23-20217)

Pettine, J. A. and D. J. Nesbitt. Emerging Methods for Controlling Hot Carrier Excitation and Emission Distributions in Nanoplasmonic Systems. Submitted to *Journal of Physical Chemistry C*. (LA-UR-23-23033)

Presentation Slides

Chen, H. Ultrafast Nanoscale Photocurrent Control and Terahertz Emission with Symmetry-Broken Optoelectronic Metamaterial. Presented at *OTST 2022*, Budapest, Hungary, 2022-06-19 - 2022-06-24. (LA-UR-22-25837)

Chen, H. Direct Generation of Terahertz Vector Beams with Symmetry-Controlled Optoelectronic Metasurfaces. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22354)

Pettine, J. A., P. Padmanabhan and H. Chen. Ultrafast Vectorial Currents in Nanoscale Symmetry-Controlled Optoelectronic Metasurfaces. Presented at *APS March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-22-31114)

Pettine, J. A. and H. Chen. Ultrafast Vectorial Currents in Nanoscale Symmetry-Controlled Optoelectronic Metasurfaces. Presented at *APS March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22353)

**Peer-reviewed*

Emergent Phenomena in Magnetically Frustrated Flourine-Electron Quantum Materials

Priscila Rosa
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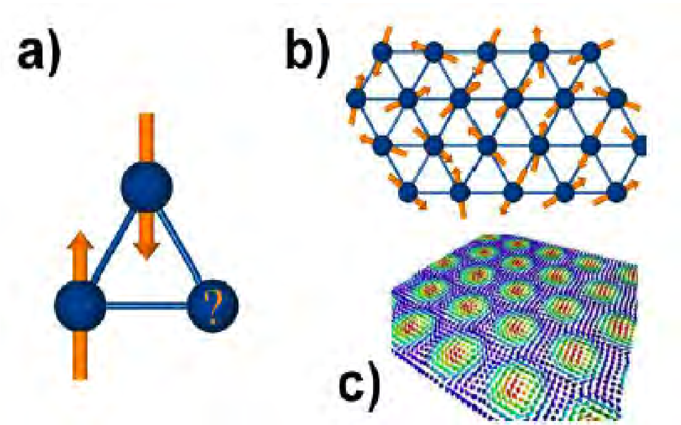


a) Frustrated spins in a triangular lattice. b) Highly entangled state known as quantum spin liquid that holds promise for quantum computing applications. c) Skyrmion lattice that holds promise for high-density memory storage.

Project Description

Magnetically frustrated quantum materials show great potential for future technologies, such as quantum computation or high-density memory storage, but identifying suitable materials with ideally frustrated magnetic interactions remains an outstanding challenge within this field. In this project, we aim at synthesizing and investigating quantum materials that minimize existing bottlenecks by specifically targeting magnetic properties of underexplored f-electron-based frustrated lattices with appropriate magnetic interactions. Two types of f-electron materials will be investigated in which quantum spin liquid ground states or spin textures are predicted to appear. Ultimately, this project will lead to predictive understanding of unusual magnetic states in the fully quantum regime as a function of chemical and electronic tunability.

Publications

Journal Articles

Bordelon, M. M., C. Girod, F. Ronning, K. Rubi, N. Harrison, J. D. Thompson, C. Dela Cruz, S. M. Thomas, E. D. Bauer and P. F. S. Rosa. Interwoven atypical quantum states in CeLiBi2. 2022. *Physical Review B*. **106** (21): 214433. (LA-UR-22-30685 DOI: 10.1103/PhysRevB.106.214433)

Presentation Slides

Bordelon, M. M. Introduction to crystalline electric fields. . (LA-UR-22-24191)

Bordelon, M. M. Tunable quantum phases in frustrated f-electron materials. Presented at *National Renewable Energy Laboratory Colloquium*, Golden (Online), Colorado, United States, 2023-02-24 - 2023-02-24. (LA-UR-23-21961)

Bordelon, M. M., C. P. M. Girod, J. D. Thompson, F. Ronning, K. Rubi, N. Harrison, R. Yamamoto, M. Hirata, S. M. Thomas, E. D. Bauer, P. Rosa, C. dela Cruz and S. Calder. Unusual magnetic order and crystalline electric fields in itinerant Cerium-based materials. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22250)

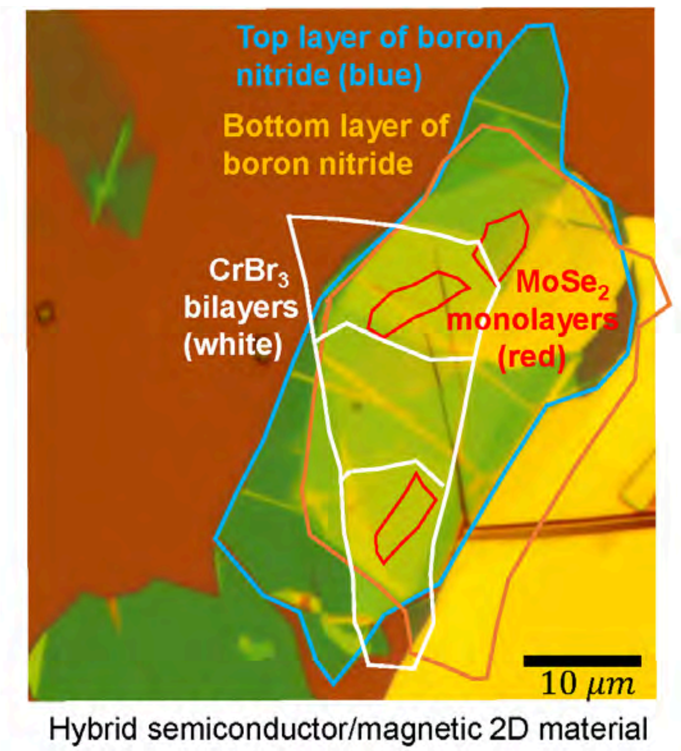
Bordelon, M. M., C. P. M. Girod, S. M. Thomas, J. D. Thompson, E. D. Bauer and P. Rosa. Unusual antiferromagnetism and field-induced transitions in tetragonal CeLiBi2. Presented at *International Conference on Strongly Correlated Electron Systems*, Campinas, Brazil, 2021-09-27 - 2021-10-02. (LA-UR-21-28184)

Rosa, P., S. M. Thomas, C. P. M. Girod, J. D. Thompson and E. D. Bauer. Unusual magnetism and field-induced transitions in Cerium-based materials. Presented at *New directions in strong correlation physics: From strange metals to topological superconductivity*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-28. (LA-UR-22-20362)

**Peer-reviewed*

Programmable Waveguides of Spin-Polarized Current with "Twisted" Moire Crystals

Scott Crooker
20210913PRD2



Microscope image of a hybrid 2D material, comprising a molybdenum diselenide (MoSe2) monolayer semiconductor on a magnetic chromium bromide (CrBr3) bilayer. The whole device is encapsulated in hexagonal boron nitride. The magnetism of the CrBr3 is 'felt' by the (otherwise nonmagnetic) MoSe2, due to the magnetic proximity effect.

Project Description

Two-dimensional (2D), atomically-thin materials are poised to revolutionize electronics and opto-electronics technologies. The most well-known example is graphene, discovered in 2004, which is a single atomic layer of carbon atoms: graphene exhibits remarkable electronic properties such as high electrical conductivity and also remarkable mechanical properties such as high strength. More recently, other 2D materials have been discovered that exhibit additional technologically useful properties, such as semiconducting behavior (which allows for light-emitting and light-detection capabilities) and also magnetism (which allows for information storage and processing). This project is focused on exploring a hybrid route towards achieving magnetic functionality in 2D semiconductors such as molybdenum diselenide (WSe2) to achieve electrically-controllable magnetism -- a longstanding goal in the broad field of semiconductor electronics, with immediate technological relevance in the areas of data storage and information processing (ie, computing).

Publications

Journal Articles

Li, X., A. C. Jones, J. Choi, H. Zhao, V. Chandrasekaran, M. T. Pettes, A. Piryatinski, N. Sinitsyn, S. A. Crooker and H. Htoon. Proximity Induced Chiral Quantum Light Generation in Strain-Engineered WSe2/NiPS3 Heterostructures. Submitted to *Nature Nanotechnology*. (LA-UR-22-20519)

Presentation Slides

Choi, J. Twist-Angle Controls Interlayer Exciton Dynamics in Transition Metal Dichalcogenide (TMD) Bilayers. Presented at *Theme Meeting at Center for Nanophase Materials Sciences in Oak Ridge National Laboratory*, Oak Ridge, Tennessee, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-23522)

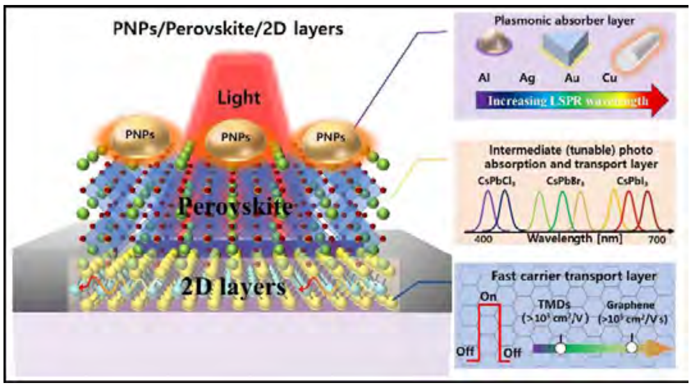
Posters

Choi, J., C. A. Lane, J. Zhu and S. A. Crooker. Asymmetric magnetic proximity interactions in MoSe2/CrBr3 van der Waals geterostructures. Presented at *Two Dimensional Electronics Beyond Graphene - Gordon Research Conference*, Manchester, New Hampshire, United States, 2022-06-12 - 2022-06-17. (LA-UR-22-25471)

**Peer-reviewed*

High-Performance Photo-Sensor/Detector by Multiplexed Heterojunction of Two-Dimensional Epitaxial Layers/Perovskites/Plasmonic Nanoparticles

Aiping Chen
20210945PRD2



The hybrid structure of UV photodetectors based on functional materials and plasmonic nanoparticles

Project Description

Photodetectors play critical roles in various optoelectronic applications. The key challenges to the practical applications are the balance between the photoresponsivity, selectivity and stability apart from the cost. This project will develop a hybrid material platform based on the engineered design of two-dimensional (2D) epitaxial layers, perovskites and plasmonic nanoparticles for high performance tunable broadband photodetectors. Such hybrid structure is deemed to take the advantage of high carrier mobility of 2D layers and superior optical absorption coefficient of perovskite, and excellent localized surface plasmon resonance of perovskite nanoparticles (PNPs). The successful development of materials and devices would provide an alternative path towards the design of high-performance photodetectors with wider spectral selectivity for advanced communication, imaging, and sensing applications. At the end of this project, we expect to optimize the plasmonic nanoparticles size and distribution in a film matrix of semi-conducting oxides or halide perovskite to achieve enhanced ultraviolet (UV) phototector performance such as fast response time and high sensitivity with low cost for high performance tunable broadband photodetector applications.

Publications

Journal Articles

Kunwar, S. Dual-step photocarrier injection by mixture layer of ZnO QDs and MoS2 NPs on hybrid PdAu NPs. Submitted to *Materials Research Bulletin*. (LA-UR-22-25124)

Kunwar, S. Super-porous Pt/CuO/Pt hybrid platform for ultra-sensitive and selective H2O2 detection. Submitted to *Applied Surface Science*. (LA-UR-22-25123)

Kunwar, S. Hybrid UV Photodetector Design Incorporating AuPt Alloy Hybrid Nanoparticles, ZnO Quantum Dots, and Graphene Quantum Dots. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-23-20268)

Kunwar, S. Protons: Critical Species for Resistive Switching in Interface-Type Memristors. 2023. *Advanced Electronic Materials*. **9** (1): 2200816. (LA-UR-23-20271 DOI: 10.1002/aelm.202200816)

*Lin, S., R. Kulkarni, R. Mandavkar, M. A. Habib, S. Burse, S. Kunwar and J. Lee. Surmounting the interband threshold limit by the hot electron excitation of multi-metallic plasmonic AgAuCu NPs for UV photodetector application. 2022. *CrystEngComm*. **24** (22): 4134-4143. (LA-UR-22-25125 DOI: 10.1039/D2CE00367H)

Lin, S., R. Mandavkar, M. A. Habib, S. Burse, T. Khalid, M. H. Joni, M. Li, S. Kunwar and J. Lee. Investigation on the AgPt and AgPd hybrid alloy nanoparticles (HANPs) for the hybrid MoS2/ZnO/HANP UV photodetector application. 2023. *Applied Surface Science*. **611** (Part A): 155559. (LA-UR-23-20269 DOI: 10.1016/j.apsusc.2022.155559)

*Lin, S., R. Mandavkar, R. Kulkarni, S. Burse, M. A. Habib, S. H. Kim, M. Li, S. Kunwar and J. Lee. MoS Nanoflake and ZnO Quantum Dot Blended Active Layers on AuPd Nanoparticles for UV Photodetectors. 2022. *ACS Applied Nano Materials*. **5** (3): 3289-3302. (LA-UR-22-20997 DOI: 10.1021/acsanm.1c03748)

Mandavkar, R., S. Lin, S. Pandit, R. Kulkarni, S. Burse, M. A. Habib, S. Kunwar and J. Lee. Hybrid SERS platform by adapting both chemical mechanism and electromagnetic mechanism enhancements: SERS of 4-ATP and CV by the mixture with GQDs on hybrid PdAg NPs. 2022. *Surfaces and Interfaces*. **33**: 102175. (LA-UR-23-20270 DOI: 10.1016/j.surfin.2022.102175)

*Pandey, P., S. Kunwar, K. Shin, M. Seo, J. Yoon, W. Hong and J. Sohn. Plasmonic Core-Shell-Satellites with Abundant Electromagnetic Hotspots for Highly Sensitive and Reproducible SERS Detection. 2021. *International Journal of Molecular Sciences*. **22** (22): 12191. (LA-UR-22-20995 DOI: 10.3390/ijms222212191)

Presentation Slides

Chen, A. Emergent Devices for Neuromorphic Computing. Presented at *EMA2023*, orlando, Florida, United States, 2023-01-17 - 2023-01-21. (LA-UR-23-20479)

Kunwar, S. Critical role of ambient moisture in resistive switching at Au/Nb:STO Schottky interface. Presented at *EMA 2023: Basic Science and Electronic Materials Meeting*, Orlando, Florida, United States, 2023-01-17 - 2023-01-22. (LA-UR-23-20403)

Kunwar, S., P. Roy, N. G. Cucciniello and A. Chen. Interface type Memristive Devices. Presented at *IMF2023*, Tel Aviv, Israel, 2023-03-27 - 2023-03-30. (LA-UR-23-23079)

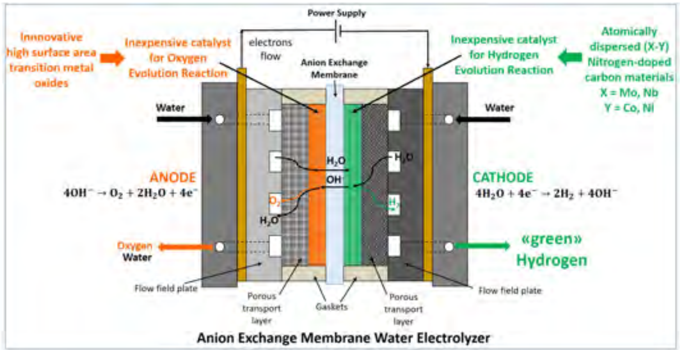
Posters

Kunwar, S. Resistive switching in Au/Nb:STO junctions: Role of ambient environment & interface quality. Presented at *Electronic Materials and Applications 2022 (EMA 2022)-Virtual Only*, Virtual Event, Nebraska, United States, 2022-01-19 - 2022-01-22. (LA-UR-23-20266)

**Peer-reviewed*

Electrocatalysts for Entirely Platinum Group Metal-Free Water Electrolyzer

Luigi Osmieri
20210953PRD3



Anion exchange membranes water electrolyzer utilizing innovative platinum group metal-free catalysts for oxygen evolution reaction (OER) at the anode and hydrogen evolution reaction (HER) at the cathode. Catalysts developed in the project will enable low-temperature and low-cost generation of "green" hydrogen using exclusively pure water.

Project Description

This project directly addresses the important national security challenge of producing "green" hydrogen using electricity from renewable sources and at a competitive cost. Production of hydrogen via water electrolysis in low temperature water electrolyzers (LTEs) is especially attractive thanks to the close to ambient operating conditions and fast startup/shutdown, enabling an effective use and storage of the intermittent electricity from renewable sources (solar, wind). Current LTEs suffer from two main drawbacks: the use of highly corrosive solutions and the need for expensive catalysts based on precious metals. Recent advancements in performance and stability of anion exchange membranes (AEM) have enabled a new alkaline membrane-based LTE technology capable of successfully competing with incumbent technologies. This project will focus on the development of high-performance and low-cost catalysts for the AEM LTEs utilizing electrocatalysts based on earth-abundant elements. It will enable the deployment a technology for “green” hydrogen generation, with the ultimate goal of facilitating the transition to new energy systems based on renewable sources and thus mitigating the effects of global warming.

Publications

Journal Articles

Osmieri, L., Y. He, H. T. Chung, G. McCool, B. Zulevi, D. A. Cullen and P. Zelenay. La-Sr-Co Oxide Catalysts for Oxygen Evolution Reaction in Anion Exchange Membrane Water Electrolyzer: The Role of Electrode Fabrication on Performance and Durability. Submitted to *Journal of Power Sources*. (LA-UR-22-30090)

Presentation Slides

Osmieri, L. Catalysts and Electrode Engineering for Affordable Low-Temperature Fuel Cells and Water Electrolyzers. . (LA-UR-22-32602)

Osmieri, L., H. Yu, P. Zelenay and D. A. Cullen . Towards Entirely Platinum Group Metal-Free Water Electrolyzers: Innovative Electrocatalysts for Oxygen Evolution and Hydrogen Evolution Reactions. Presented at *Electrochemical Society (ECS) Spring Meeting*, Vancouver, Canada, 2022-05-29 - 2022-06-02. (LA-UR-22-24964)

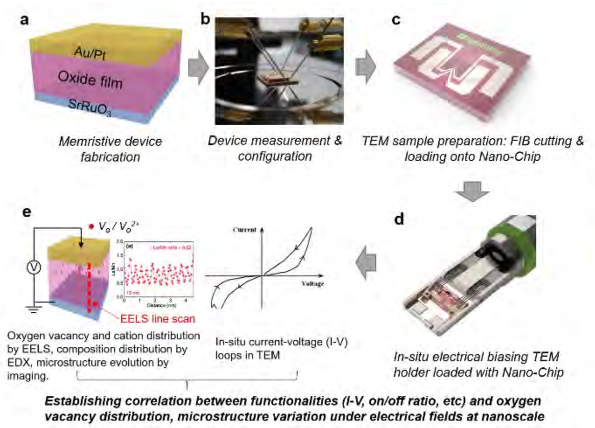
Osmieri, L., Y. He, I. R. Ortega, J. D. Jernigen, H. Yu, D. A. Cullen and P. Zelenay. PGM-free Catalysts and Electrodes for Anion Exchange Membrane Water Electrolyzers. Presented at *Electrochemical Society (ECS) Fall Meeting*, Atlanta, Georgia, United States, 2022-10-09 - 2022-10-13. (LA-UR-22-30091)

Osmieri, L. and P. Zelenay. Lessons learnt about impact of different synthesis and testing variables on OER catalysts performance. Presented at *ElectroCat 2.0 semiannual in person meeting*, Santa Fe, New Mexico, United States, 2023-02-13 - 2023-02-14. (LA-UR-23-21216)

**Peer-reviewed*

In Operando Study of Resistive-Switching Devices at Nanoscale

Aiping Chen
20210954PRD3



In-situ observation of memristive switching at nanoscale in operando. These experiments will for the first time allow the team to directly observe oxygen vacancies migrations process in-situ memristors during operation at the nanoscale in electron microscopy. The revealed underlying operation mechanisms will allow the team to design better memory devices and neuromorphic computing devices.

Project Description

Resistive-switching (RS) observed in a variety of transitional-metal oxides is of great research interest since it opens up enormous opportunities in next-generation integrated electronics such as nonvolatile memory, and neuromorphic computing devices etc. Recent advances have shown a new interface-type RS devices with lower operation current and more reliable switching repeatability could revolutionize data storage and neuromorphic computing. However, the mechanisms of such interface-type devices are not clearly understood, which hinders the design and application of the new interface-type devices for memory and neuromorphic computing. This work, if successful, will for the first time allow us to directly observe oxygen vacancies migrations process in-situ in memristors during operation at the nanoscale in electron microscopy. The physical principles discovered in this work will be critical to design memristor devices for next generation memory devices and neuromorphic computing. Developing advanced microelectronic devices underpins the Department of Energy-Basic Energy Science research interests in “Microelectronics” and “Beyond Moore”.

Publications

Journal Articles

Li, Y., W. Wang, D. Zhang, M. Baskin, A. Chen, S. Kvatinsky, E. Yalon and L. Kornblum. Scalable Al2O3-TiO2 Conductive Oxide Interfaces as Defect Reservoirs for Resistive Switching Devices. 2022. *Advanced Electronic Materials*. 2200800. (LA-UR-22-30963 DOI: 10.1002/aelm.202200800)

*Roy, P., S. Kunwar, D. Zhang, D. Chen, Z. Corey, B. X. Rutherford, H. Wang, J. L. MacManus-Driscoll, Q. Jia and A. Chen. Role of Defects and Power Dissipation on Ferroelectric Memristive Switching. 2022. *Advanced Electronic Materials*. **8** (6): 2101392. (LA-UR-22-23966 DOI: 10.1002/aelm.202101392)

*Rutherford, B. X., B. Zhang, M. Kalaswad, Z. He, D. Zhang, X. Wang, J. Liu and H. Wang. Tunable Three-Phase Co-CeO2-BaTiO3 Hybrid Metamaterials with Nano-Mushroom-Like Structure for Tailorable Multifunctionalities. 2022. *ACS Applied Nano Materials*. **5** (5): 6297-6304. (LA-UR-22-23968 DOI: 10.1021/acsanm.2c00394)

Song, J., D. Zhang, P. Lu, H. Wang, X. Xu, M. Meyerson, S. Rosenberg, J. Deitz, J. Liu, X. Wang, X. Zhang and H. Wang. Anisotropic Optical and Magnetic Response in Self-Assembled Tin-Cofe2 Nanocomposites. Submitted to *SSRN Electronic Journal*. (LA-UR-22-31787)

Song, J., D. Zhang, P. Lu, H. Wang, X. Xu, M. Meyerson, S. Rosenberg, J. Deitz, J. Liu, X. Wang, X. Zhang and H. Wang. Anisotropic optical and magnetic response in self-assembled TiN-CoFe2 nanocomposites. 2023. *Materials Today Nano*. **22**: 100316. (LA-UR-23-21211 DOI: 10.1016/j.mtnano.2023.100316)

Zhang, D., X. Gao, J. Lu, P. Lu, J. Deitz, J. Shen, H. Dou, Z. He, Z. Shang, C. A. Wade, X. Zhang, A. Chen and H. Wang. Novel self-assembled two-dimensional layered oxide structure incorporated with Au nanoinclusions towards multifunctionalities. 2022. *Nano Research*. (LA-UR-22-28356 DOI: 10.1007/s12274-022-4663-1)

*Zhang, Y., D. Zhang, J. Liu, P. Lu, J. Deitz, J. Shen, Z. He, X. Zhang and H. Wang. Self-assembled HfO2-Au nanocomposites with ultra-fine vertically aligned Au nanopillars. 2022. *Nanoscale*. **14** (33): 11979-11987. (LA-UR-22-28353 DOI: 10.1039/D2NR03104C)

Presentation Slides

Chen, A. Emergent Devices for Neuromorphic Computing. Presented at *EMA2023*, orlando, Florida, United States, 2023-01-17 - 2023-01-21. (LA-UR-23-20479)

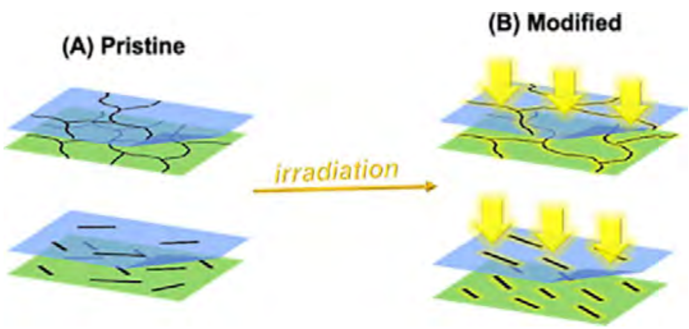
Zhang, D., J. Lu, X. Gao, P. Lu, J. Shen, H. Dou, Z. He and H. Wang. Reveal of Magnetic Domains and Tunable Supercell Structures in Two-dimensional Layered Oxide Thin Film via Differential Phase Contrast Imaging and Atomic-resolution STEM\xc2\xa0. Presented at *Microscopy and Microanalysis 2022*, Portland, Oregon, United States, 2022-07-31 - 2022-08-04. (LA-UR-22-28355)

Zhang, D., K. Ssennyimba, Z. Hughes, M. Zachman, C. Somodi, Y. Sharma, B. Paudel, B. Freiman, S. Kunwar, A. Mazza, P. Roy and A. Chen. A novel combinatorial approach to the synthesis of a lead-free ferroelectric relaxor system. Presented at *Electronic Materials and Applications*, Orlando, Florida, United States, 2023-01-17 - 2023-01-20. (LA-UR-23-20559)

**Peer-reviewed*

Defect Engineering of Two-Dimensional Materials by Ion Irradiation

Jinkyoung Yoo
20210965PRD4



Scheme of ion beam irradiation onto two-dimensional materials to modify physical characteristics. The project aims at development of post-processing techniques for next-generation semiconductor devices based on atomically thin nanomaterials.

Project Description

Advances in electronic and photonic devices are requiring novel nanomaterials as building blocks. Atomically thin semiconducting materials are being considered as promising for the next-generation devices. However, controlling physical characteristics of atomically thin materials for devices is difficult. The project aims at development of ion beam-based processing techniques to modify atomically thin materials in precise manner. Demonstration of durable devices is expected by understanding correlation between ion beam irradiation and irradiated materials' characteristics. The combination of fundamental understanding of materials behaviors and device demonstration can make broad impacts on various national security mission areas in which semiconductor devices are required for controlling systems at extreme conditions, such as space, and detecting signals.

Publications

Journal Articles

Wang, X., M. T. Pettes, Y. Wang, J. Zhu, R. Dhall, C. Song, A. C. Jones, J. Ciston and J. Yoo. Edge states induced enhancement of exciton-to-trion conversion in proton irradiated WS2. Submitted to *Nature Communications*. (LA-UR-22-29441)

Presentation Slides

Wang, X. Nucleation of Hexagonal Germanium Grains on Defect Engineered MoS2\xc2\xa0Monolayers. Presented at *Materials Research Society (MRS) Fall Meeting and Exhibit*, Boston, Massachusetts, United States, 2022-11-27 - 2022-12-02. (LA-UR-22-32289)

Wang, X., Y. Wang, H. Htoon, M. T. Pettes, A. C. Jones and J. Yoo. Control of Optical Properties via Ion Irradiation of Two-Dimensional Transition Metal Dichalcogenides. Presented at *MRS Spring*, Honolulu, Hawaii, United States, 2022-05-09 - 2022-05-13. (LA-UR-22-24190)

Yoo, J. Quantum structures prepared by remote epitaxy over two-dimensional transition metal dichalcogenides. Presented at *Advanced Epitaxy for Freestanding Membranes and 2D Materials*, Boston, Massachusetts, United States, 2022-07-06 - 2022-07-06. (LA-UR-22-25682)

**Peer-reviewed*

Advancing Understanding and Prediction of Ligand-Coated Actinide Clusters

Ping Yang
20210966PRD4

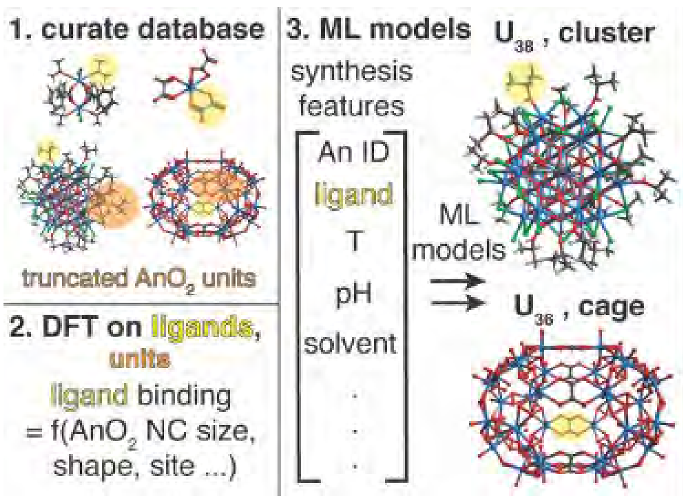


Diagram illustrating the three key steps of the proposed project. Step 1 is to curate all molecular and nanocluster (NC) actinide structures from published databases, Step 2 is to understand ligand-actinide dinging at the NC surfaces, and Step 3 is to include experimental nanocluster synthetic conditions to predict the topology of actinide NCs. This project will advance in understanding and accelerated methods towards prediction of actinide oxide cluster structures with ligands.

Project Description

Nanoscale materials bearing heavy elements, such as thorium and uranium oxide nanoparticles play an increasingly important role in many stages of the nuclear fuel cycle, from recycling spent nuclear fuel during the precipitation step, to high temperature (T) processing of actinide mixture, to mixed oxide fuels. The formation and stability of actinide nanoparticles are also vital to long-term management of nuclear waste sites due to leaching/environmental concerns. Recent work illustrated how surface energies control the morphology of large nanoparticles via Wulff construction. However, the energetics of small to medium sized Anoctamin 2 (AnO2) nanoclusters (NCs) in the presence of different ligands remains unclear at the atomic level as these NCs do not resemble their bulk nor molecular structures due to strong metal-ligand binding interactions. AnO2 NCs typically consist of particles built of AnO2 building blocks stabilized by ligands into either colloidal cages or clusters. This project will advance in understanding and accelerated methods towards prediction of actinide oxide cluster structures with ligands.

Publications

Journal Articles

Taylor, M. G., D. J. Burrill, J. Janssen, E. R. Batista, D. Perez and P. Yang. Architector: high-throughput cross-periodic table 3D complex builder. Submitted to *Nature Communications*. (LA-UR-22-25834)

Presentation Slides

Taylor, M. G. Architector: towards learning across the mononuclear periodic table. Presented at *Machine Learning and Informatics for Chemistry and Materials*, Telluride, Colorado, United States, 2022-10-03 - 2022-10-07. (LA-UR-22-30196)

Taylor, M. G. Architector: high-throughput generation of f-block molecular complexes. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-03. (LA-UR-23-21730)

Taylor, M. G., D. J. Burrill, J. Janssen, E. R. Batista, D. Perez and P. Yang. Learning actinide-ligand binding motifs and structure from organometallic structural databases. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28791)

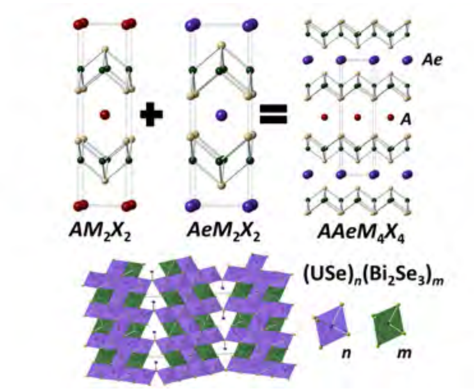
Other

Taylor, M. G. and P. Yang. XTB-relaxed, experimentally derived d-Block mononuclear complexes. Dataset. (LA-UR-22-29779)

**Peer-reviewed*

Emergent Quantum States through Quantum Confinement in Flourine-Electron Materials

Eric Bauer
20210967PRD4



This work will focus on the growth and characterization of high quality single crystals of low dimensional f-electron quantum materials. Intrinsic heterostructures of AAeM4X4 (A = 4f/5f element; Ae = Ca, Sr, Ba; M = transition metal; X = P, As, Si, Ge) and (USe)n(Bi2Se3)m, will be respectively built from superconducting AM2X2 layers and spacer layers of AeM2X2 building blocks (top) and binary USe and Bi2Se3 stacked subunits (bottom). This work will lead to the exploration of new quantum states which is significant to the fields of superconductivity, magnetism, and topology.

Project Description

This project will discover new low-dimensional rare earth and actinide quantum materials and investigate their novel and interesting quantum states. Quantum materials have great potential for use in future architectures for quantum computing and quantum information science to ensure the Nation's energy security.

Publications

Presentation Slides

Weiland, A. C., S. S. Fender, F. Ronning, J. D. Thompson, E. D. Bauer, S. M. Thomas and P. Rosa. Correlating Tc and Crystallographic Parameters in UTe2. Presented at *Chirality, Topology, and Unconventional Superconductivity in Sr2RuO4 and UTe2*, Santa Fe, New Mexico, United States, 2021-10-28 - 2021-10-30. (LA-UR-21-30512)

Weiland, A. C., S. S. Fender, M. M. Bordelon, F. Ronning, J. D. Thompson, E. D. Bauer, S. M. Thomas and P. Rosa. The Effects of Annealing in UTe2. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-15 - 2022-03-19. (LA-UR-22-22016)

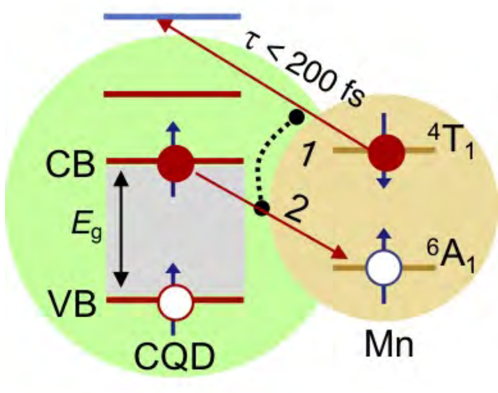
Posters

Weiland, A. C., P. Rosa, S. S. Fender, B. L. Scott, F. Ronning, J. D. Thompson, E. D. Bauer and S. M. Thomas. A Crystallographic Study of UTe2. Presented at *NEW DIRECTIONS IN STRONG CORRELATION PHYSICS: FROM STRANGE METALS TO TOPOLOGICAL SUPERCONDUCTIVITY*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-29. (LA-UR-22-20422)

**Peer-reviewed*

High-Efficiency Photoemission from Quantum Dots Enabled by Ultrafast Spin Exchange

Victor Klimov
20220699PRD1



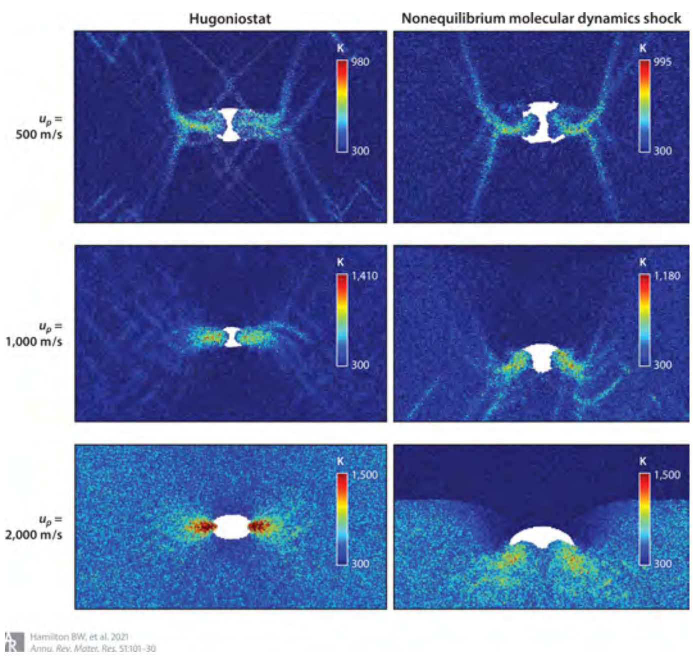
Photoemission due to spin-exchange Auger ionization is triggered by absorption of two low-energy photons with energies greater than the band-gap (Eg). This leads to generation of two excitons, one residing in the colloidal quantum dots (CQD) and the other, on the manganese (Mn) ion. Auger ionization is achieved due to spin-exchange recombination of this 'hybrid bi-exciton' during which the collapse of the excited Mn state is accompanied by ejection of the energy-accepting electron from the CQD.

Project Description

Photocathodes are essential components of numerous devices from photomultipliers and night-vision tubes to electron microscopes and free-electron lasers. Their operation is based on the effect of 'photoemission' wherein a material emits electrons upon exposure to high-energy (typically, ultraviolet (UV)) photons. The objective of this project is to explore an alternative process – ultrafast spin-exchange Auger ionization– for achieving highly efficient photoemission with visible and even infrared illumination. This effect emerges as a result of confinement-enhanced spin-exchange interactions in magnetically-doped colloidal quantum dots. It can enable a new type of inexpensive photocathodes that will combine high photoelectron yields with exceptional robustness stemming from the short-range character of spin-exchange interactions, which makes them insensitive to the external environment.

Influence of Intra-Molecular Mechanical Strain on Solid State Reaction Pathways

Timothy Germann
20220705PRD1



Shock compression of molecular solids produces local strain and temperature conditions that lead to complex molecular deformations and covalent mechanochemistry, such as the shock-to-detonation transition in energetic materials. Image Credit: Hamilton et al, Annual Reviews of Materials Research 51, 101 (2021).

Project Description

The objective of this research effort is to develop detailed understanding of the relationship between mechanical deformations of covalent molecules and the reaction pathways they undergo and the resulting reaction kinetics. Particular focus will be placed on simulating loading of complex and realistic material microstructures to enable the mapping of molecular deformations. Reactive and ab initio molecular dynamics (MD) simulations will be utilized to explore many-bodied molecular deformations effects on chemical reactivity for a variety of relevant materials such as high explosive (HE) and polymer-based materials.

Publications

Journal Articles

Hamilton, B. W., M. P. Kroonblawd, J. Macatangay, H. K. Springer and A. Strachan. Intergranular Hotspots: A Molecular Dynamics Study on the Influence of Compressive and Shear Work. Submitted to *Journal of Physical Chemistry C*. (LA-UR-23-21420)

Hamilton, B. W., P. Yoo, M. N. Sakano, M. M. Islam and A. Strachan. High Pressure and Temperature Neural Network Reactive Force Field for Energetic Materials. Submitted to *Journal of Chemical Physics*. (LA-UR-23-21289)

Hamilton, B. W. and A. Strachan. Rapid Activation of Non-Oriented Mechanophores via Shock Loading and Spallation. Submitted to *Physical Review Materials*. (LA-UR-22-32416)

Hamilton, B. W. and T. C. Germann. Energy localization efficiency in 1,3,5-trinitro-2,4,6-triaminobenzene pore collapse mechanisms. 2023. *Journal of Applied Physics*. **133** (3): 035901. (LA-UR-22-31052 DOI: 10.1063/5.0133983)

Hamilton, B. W. and T. C. Germann. Influence of Pore Surface Structure and Contents on Shock Induced Collapse and Energy Localization. Submitted to *Journal of Physical Chemistry C*. (LA-UR-23-21096)

Hamilton, B. W. and T. C. Germann. Interplay of Mechanochemistry and Material Processes in the Graphite to Diamond Phase Transformation. Submitted to *Physical Review Letters*. (LA-UR-23-21258)

Lafourcade, P., J. Maillet, J. Roche, M. N. Sakano, B. W. Hamilton and A. Strachan. Multiscale reactive model for 1,3,5-triamino-2,4,6-trinitrobenzene inferred by reactive MD simulations and unsupervised learning. Submitted to *Journal of Physical Chemistry C*. (LA-UR-23-23237)

Presentation Slides

Hamilton, B. W. Project Review t22_he_mechanochem. . (LA-UR-23-22866)

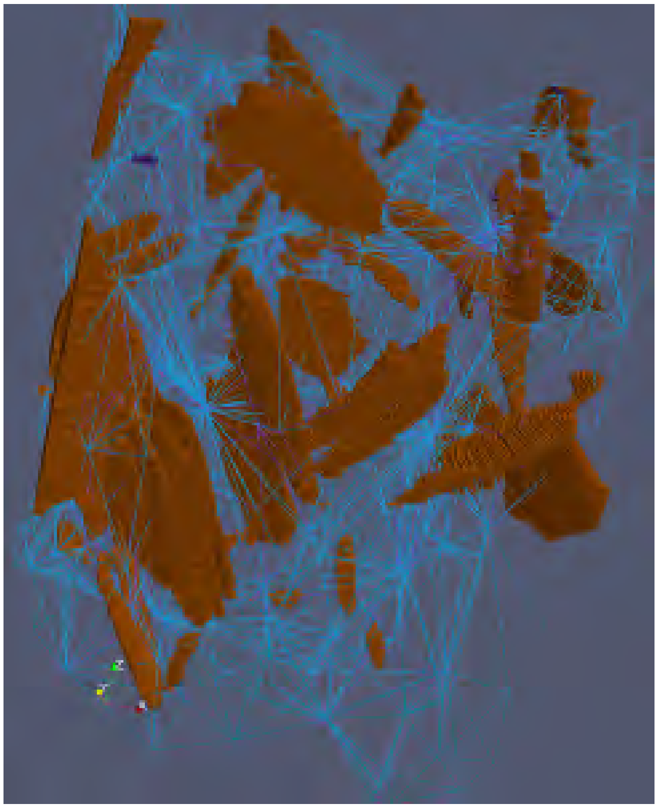
Hamilton, B. W. Using Machine Learning to Understand the Key Mechanisms in Shockwave Initiation of Energetic Materials. Presented at *Los Alamos National Laboratory Science in "3"*, Los Alamos, New Mexico, United States, 2023-06-28 - 2023-06-28. (LA-UR-23-23121)

Hamilton, B. W. and T. C. Germann. Efficiency of Energy Localization in Hotspot Formation for Complex Pore Collapse Mechanisms. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-02-10. (LA-UR-23-22248)

**Peer-reviewed*

Development/Application of 4D-Stem and 3D Electron Backscatter Diffraction to Connect Stresses with Microstructural Evolution in Materials at the Nanometer and Macroscopic Length Scales

Laurent Capolungo
20220790PRD2



Three-dimensionally (3D) reconstructed image of a twin network in pure Ti. This project will develop two emergent experimental techniques that address critical aspects of understanding and predicting material evolution under mechanical loading.

Project Description

The ability to reliably and consistently predict how structural metals will perform during operation is critical to Weapon Program as well as the Nuclear Energy Program. However, the materials response under intense radiation, temperature, and complicated loading such as shock loading requires more advanced experimental techniques to fully capture and correlate the external environments, internal states, and the resulting material response from the atomic level to the structural level. In this project, emergent experimental techniques that address two critical aspects of understanding and predicting material evolution under mechanical loading will be matured. Specifically electron microscopy techniques will be extended to characterize in situ the evolution of driving forces for the activation of deformation in complex metals. Second, a new method will be stood up to allow for the reconstruction of three dimensional deformed microstructures.

Publications

Journal Articles

Vo, H. T., D. Frazer, A. A. Kohnert, S. Teysseyre, S. J. Fensin and P. Hosemann. Role of low-level void swelling on channel suppression and intergranular cracking in a 33 dpa neutron-irradiated 304 stainless steel. Submitted to *Materials & Design*. (LA-UR-22-32375)

Vo, H. T., S. Pal, N. Almirall, S. Tumey, G. R. Odette, S. Maloy and P. Hosemann. Dose and dose rate effects on the microstructural and mechanical stability of long-range ordered precipitates in Inconel 718. 2023. *Materials Science and Engineering: A*. 144916. (LA-UR-22-31172 DOI: 10.1016/j.msea.2023.144916)

Presentation Slides

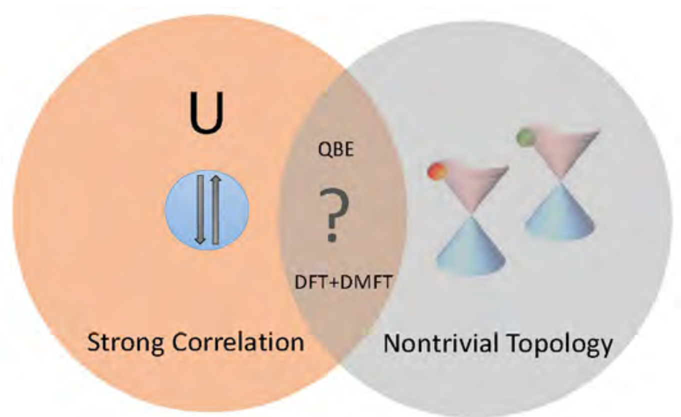
Vo, H. T., K. Q. Dang, F. Teng, M. M. Schneider, B. P. Eftink, S. Maloy, J. D. Tucker, L. Capolungo and P. Hosemann. Understanding the Influence of LRO precipitates on Plastic Stability and Deformation Mode in FCC Ni2Cr Alloy. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-23. (LA-UR-23-22719)

Vo, H. T., K. Q. Dang, F. Teng, M. M. Schneider, B. P. Eftink, S. Maloy, J. Tucker, L. Capolungo and P. Hosemann. Understanding the Influence of LRO precipitates on Plastic Stability and Deformation Mode in FCC Ni2Cr Alloy. Presented at *Materials Science & Technology (MS&T) Technical Meeting*, Pittsburgh, Pennsylvania, United States, 2022-10-09 - 2022-10-12. (LA-UR-22-30318)

**Peer-reviewed*

Anomalous Transport in Correlated Topological Materials

Jianxin Zhu
20220792PRD2



Although the transport properties of uncorrelated topological materials have been extensively investigated, understanding the effect of electronic correlation on transport in correlated topological materials has yet to be explored. Strong correlation can bring about a rich selection of emergent quantum states and a significant tunability. The quantum Boltzmann formalism (QBE) including multi-band effect as well as correlation effect and the dynamical mean-field theory combined with density functional theory (DFT+DMFT) framework will shed light on the interplay between nontrivial topology (e.g., Weyl semimetals with two opposite chirality nodes) and electronic correlation (U), pictured here. [Image credit: Los Alamos National Laboratory]

Project Description

At the heart of modern quantum materials research is exploring the macroscopic manifestations of quantum mechanics that give rise to coherent and topologically protected phenomena. These materials hold a huge promise for next-generation quantum devices for energy and information. The grand challenge is to discover, identify, and ultimately control these materials for a targeted property or functionality. The scientific goal of this research is to unravel the role of strong correlation and topology in the transport properties of quantum materials, which will provide, together with electronic structure, an unambiguous identification of the electronic state in the materials. By incorporating materials specific into the theoretical modeling, the research will make a direct connection with some of the most exciting experimental signatures. The research addresses the Department of Energy (DOE) Quantum Materials Basic Needs in the Priority Research Direction: Control and exploit electronic interactions and quantum fluctuations for design of bulk materials with novel functionality.

Publications

Journal Articles

Ghosh, S., A. Sahoo and S. Nandy. Theoretical investigations on Kerr and Faraday rotations in topological multi-Weyl Semimetals. Submitted to *Physical Review B*. (LA-UR-22-29847)

Nag, T., S. K. Das, C. Zeng and S. Nandy. Third-order Hall effect in the surface-states of topological insulator. Submitted to *Physical Review B*. (LA-UR-22-29522)

Presentation Slides

Nandy, S., C. A. Lane and J. Zhu. Weyl-Hubbard System: A Platform to Investigate Interplay between Topology and Correlation. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22272)

Posters

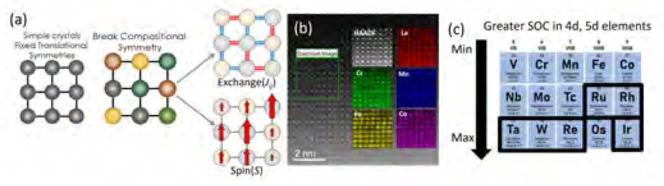
Nandy, S., C. A. Lane and J. Zhu. Quantum Hall Effect in Weyl-Hubbard System: Interplay Between Topology and Correlation. Presented at *Topology, Symmetry and Interactions in Crystals: Emerging Concepts and Unifying Themes*, Santa Barbara, California, United States, 2023-04-03 - 2023-04-06. (LA-UR-23-23211)

**Peer-reviewed*

High Entropy Oxides for Quantum Applications

Aiping Chen

20220796PRD2



Adding the local symmetry breaking of high entropy oxides (a) and applying it to spin and exchange, relevant to magnetism, leads to broad tunability in high entropy oxides. (b) shows the complete mixing of many elements on the single crystal lattice. (c) shows some candidate materials in choosing elements with large spin orbit coupling.

Project Description

The fundamental limitation on innovation in quantum, energy, and green technologies is the ability to synthesize materials which meet the demands of those applications. Classical methods in materials synthesis, which require the inherent internal energy of the system to be compatible with the enthalpic energy at which the material can be synthesized, fall short of these benchmarks. In a new strategy for Los Alamos National Laboratory, we propose to use entropy stabilization which allows by chaotically populating sites a lattice with many different elements in place of one. The entropy of the system allows for synthesis of materials from which the inherent, internal energy would be physically impossible to create by other means. In a first step, we focus on candidates for quantum materials hosting rich magnetic and electronic phases which are pivotal to quantum information sciences and quantum computing applications. In doing so we will harness the identified tunable magnetic phase of high entropy oxides in advancing the ability to transport the spins of electrons. This will address the device needs of spin-based electronics (spintronics) - a clear improvement on conventional charged based devices.

Publications

Journal Articles

Mazza, A. Disorder and hydrogenation in graphene nanopowder revealed by complementary X-ray and neutron scattering. 2023. *Carbon*. (LA-UR-23-21177 DOI: 10.1016/j.carbon.2023.02.005)

Mazza, A. R., E. Skoropata, J. Lapano, M. A. Chilcote, C. Jorgensen, N. Tang, Z. Gai, M. Brahlek, D. A. Gilbert and T. Z. Ward. Hole doping in compositionally complex correlated oxide enables tunable exchange biasing. Submitted to *Physical Review Applied*. (LA-UR-22-29556)

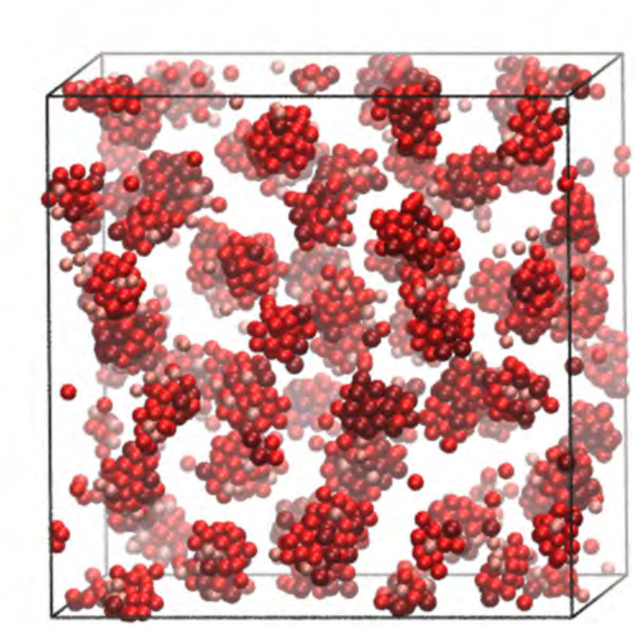
Mazza, A. R., S. R. Acharya, P. Wasik, J. Lapano, J. Li, B. L. Musico, V. Keppens, A. F. May, M. Brahlek, C. Mazzoli, J. Pelliciari, V. Bisogni, V. R. Cooper and T. Z. Ward. Variance induced decoupling of spin, lattice, and charge ordering in perovskite nickelates. 2023. *Physical Review Research*. **5** (1): 013008. (LA-UR-22-29555 DOI: 10.1103/PhysRevResearch.5.013008)

Rimal, G., A. R. Mazza, M. Brahlek and S. Oh. Diffusion-assisted molecular beam epitaxy of CuCrO thin films. 2022. *Journal of Vacuum Science & Technology A*. **40** (6): 060401. (LA-UR-22-31878 DOI: 10.1116/6.0002151)

**Peer-reviewed*

Overcoming the Curse of Dimensionality to Predict Chemical Reactivity

Beth Lindquist
20180758PRD4



Machine learning and statistical inference tools have made a significant impact across many areas of statistical mechanics. For example, in the work completed thus far on the project, these techniques have enabled 1) efficient discovery of physically realizable models that are predicted to self-assemble into complex microstructures as well as 2) the detection of phase transitions in non-equilibrium systems. The figure shows an image from a simulation that self-assembles into an equilibrium cluster fluid, where the model parameters are optimized using statistical inference methods.

Project Description

This project aims to provide a critical component of an equation of state (EOS) that is typically missing from atomistic modeling. Such work will be directly applied to high explosives (HE) equation of state modeling. This can be used to understand many important issues confronting the stockpile, such as understanding and predicting the behavior and performance of HE. This will be critical for new formulations or aged HE materials.

Technical Outcomes

Non-equilibrium processes play a role in material aging, the behavior of high explosives, and biological processes. However, these problems are challenging to investigate with established theoretical tools. The project's goal was to develop a mapping between a single non-equilibrium system and a family of equilibrium systems, the latter of which are easier to study with available computational strategies. The project successfully developed and refined several such mapping strategies to facilitate the study of non-equilibrium phenomena.

Publications

Journal Articles

*Howard, M. P., R. B. Jadrich, B. A. Lindquist, F. Khabaz, R. T. Bonnecaze, D. J. Milliron and T. M. Truskett. Structure and phase behavior of polymer-linked colloidal gels. 2019. *The Journal of Chemical Physics*. **151** (12): 124901. (LA-UR-19-26202 DOI: 10.1063/1.5119359)

*Jadrich, R. B., B. A. Lindquist and T. M. Truskett. Treating random sequential addition via the replica method. 2022. *The Journal of Chemical Physics*. **157** (8): 84116. (LA-UR-22-23178 DOI: 10.1063/5.0096276)

Lindquist, B. A. Connecting Inverse Design with Experimentally Relevant Models. Submitted to *Journal of Physics: Conference Series*. (LA-UR-20-21571)

*Lindquist, B. A. Inverse design of equilibrium cluster fluids applied to a physically informed model. 2021. *The Journal of Chemical Physics*. **154** (17): 174907. (LA-UR-21-21954 DOI: 10.1063/5.0048812)

*Lindquist, B. A., R. B. Jadrich, M. P. Howard and T. M. Truskett. The role of pressure in inverse design for assembly. 2019. *The Journal of Chemical Physics*. **151** (10): 104104. (LA-UR-19-25001 DOI: 10.1063/1.5112766)

Lindquist, B. A. and A. Rajasekaran. On the feasibility of ordered mesophase self-assembly with a physically motivated interaction potential. Submitted to *Journal of Chemical Physics*. (LA-UR-22-30765)

*Sherman, Z. M., M. P. Howard, B. A. Lindquist, R. B. Jadrich and T. M. Truskett. Inverse methods for design of soft materials. 2020. *The Journal of Chemical Physics*. **152** (14): 140902. (LA-UR-20-20466 DOI: 10.1063/1.5145177)

*Spencer, J. A., D. P. Shutt, S. K. Moser, H. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Distinguishing viruses responsible for influenza-like illness. 2022. *Journal of Theoretical Biology*. **545**: 111145. (LA-UR-21-27457 DOI: 10.1016/j.jtbi.2022.111145)

Presentation Slides

Jackson, J. M. and M. J. Monreal. GAIN: Neutron Beam Dilatometry for Molten Salt Density Measurments. Presented at *NE-43 Molten Salt Chemistry PIs Meeting*, Virtual, New Mexico, United States, 2021-06-28 - 2021-06-29. (LA-UR-21-26025)

Lindquist, B. A. Using Statistical Inference to Discover Interactions for Colloidal Self-Assembly. Presented at *Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23041)

Lindquist, B. A. Statistical Inference of Equilibrium Statistical Mechanical Models. Presented at *33rd Annual CSP Workshop: Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, Georgia, United States, 2020-02-17 - 2020-02-21. (LA-UR-20-21358)

Lindquist, B. A. Using Inverse Design to Facilitate Colloidal Self-Assembly. . (LA-UR-21-25905)

Lindquist, B. A. Self-Assembly of gels, clusters, and other modulated phases via a physically informed model. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, San Diego, California, United States, 2022-03-20 - 2022-03-24. (LA-UR-22-22571)

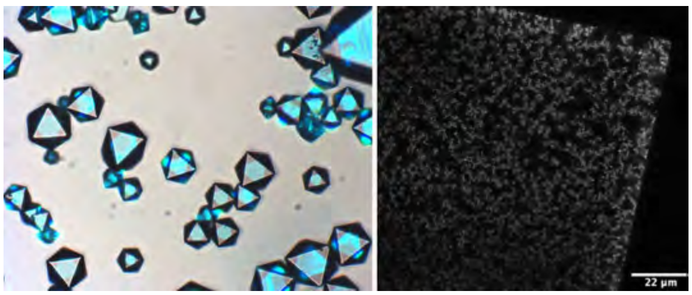
Lindquist, B. A. Using Inverse Design to Facilitate Colloidal Self-Assembly. Presented at *Materials Capability Review*, Los Alamos, New Mexico, United States, 2022-06-20 - 2022-06-23. (LA-UR-22-25520)

Lindquist, B. A. and R. B. Jadrich. Chemical Bonding in High Explosives. Presented at *ACS Fall 2021: Resilience of Chemistry*, Atlanta, Georgia, United States, 2021-08-22 - 2021-08-26. (LA-UR-21-28255)

**Peer-reviewed*

A Novel "Three-in-One" Metal Organic Framework-Based Platform For Nanoparticle Encapsulation and Organization

Ekaterina Dolgopolova
20190620PRD1



(Left) Metal-organic framework (MOF) crystals showing faceting indicative of their underlying crystal structure prepared using newly established growth reactors and protocol for enhanced crystallinity and size. (Right) Image extracted from an image-series obtained via scanning fluorescence microscopy while optically "slicing" through a three-dimensional MOF-quantum dot (QD) composite crystal to reveal incorporation of light-emitting QDs (bright spots) throughout the MOF structure.

Project Description

New and improved light-emitting, light-directing and light-transmitting materials are needed to support advanced technologies that underpin economic competitiveness, e.g., Information Science and Technology, as well as global security, e.g., via enabling new tools for improved Remote Sensing for Nuclear Nonproliferation and Counterproliferation, new materials for scintillation and radiation detection for Nuclear Nonproliferation and Counterproliferation, new strategies for Information Collection, Surveillance, and Reconnaissance, and new sensors/detectors for Chemical and Biological Weapons and Defense. The proposed work involves the development of novel, flexible photonic materials.

Technical Outcomes

This project explored the fabrication of hybrid organic-inorganic, functional materials via metal-organic framework (MOF) and nanocrystal co-assembly. In doing so, it yielded new photonic materials and enabled the establishment of new Los Alamos National Laboratory capabilities in nanomaterial assembly, two-dimensional MOF manipulation, in situ characterization of nucleation and growth kinetics, and synthesis/assembly automation.

Publications

**Peer-reviewed*

Journal Articles

Dolgopolova, E., D. Li, S. T. Hartman, J. D. Watt, C. Rios, J. Hu, R. K. Kukkadapu, J. L. Casson, R. Bose, A. V. Malko, A. V. Blake, S. A. Ivanov, O. Roslyak, A. Piryatinski, H. Htoon, H. Chen, G. Pilania and J. A. Hollingsworth. Strong Purcell Enhancement at Telecom Wavelengths Afforded by Spinel Fe3O4 Nanocrystals with Size-Tunable Plasmonic Properties. Submitted to *Nanoscale Horizons*. (LA-UR-22-31497)

Presentation Slides

Dolgopolova, E. and J. A. Hollingsworth. Alternative plasmonic nanomaterials as building blocks for Purcell-enhanced emission in the infrared. Presented at *2020 Spring ACS National Meeting, COLL Virtual Technical Symposium*, Los Alamos, New Mexico, United States, 2020-03-22 - 2020-03-24. (LA-UR-20-22500)

Dolgopolova, E. and J. A. Hollingsworth. Alternative nanomaterials with size-dependent plasmonic properties for Purcell-enhanced emission in the infrared. Presented at *ACS Fall 2020 Virtual Meeting*, San Francisco, California, United States, 2020-08-16 - 2020-08-16. (LA-UR-20-26512)

Dolgopolova, E. and J. A. Hollingsworth. Shooting for the Stars: Opening New Dimensions for Metal-Organic Frameworks. Presented at *Center for Space and Earth Science Symposium*, Los Alamos, New Mexico, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28567)

Dolgopolova, E. and J. A. Hollingsworth. Plasmonic spinel oxide nanocrystals afford Purcell-enhanced emission in the infrared. Presented at *ACS Spring 2021*, Online, New Mexico, United States, 2021-04-04 - 2021-04-30. (LA-UR-21-23397)

Dolgopolova, E. and J. A. Hollingsworth. Controlled growth of metal-organic frameworks in gels. Presented at *ACS Spring Meeting 2021*, Online, New Mexico, United States, 2021-04-04 - 2021-04-30. (LA-UR-21-23396)

Posters

Dolgopolova, E., D. Li, J. D. Watt, G. Pilania, C. Ocampo, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Alternative Plasmonic Nanomaterials for Purcell-Enhanced Emission in the Infrared Region. Presented at *CINT Annual Meeting*, Online, New Mexico, United States, 2020-09-21 - 2020-09-24. (LA-UR-20-27165)

Dolgopolova, E., J. S. Mohar, Y. Kim, G. Pilania, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Semiconductors Helping Semiconductors: Alternative Plasmonic Nanomaterials as Building Blocks for Purcell-enhanced Emission. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29475)

Novel X-ray Imaging to Unlock the Potential of Antiferromagnetic Materials

Adra Carr
20190623PRD2

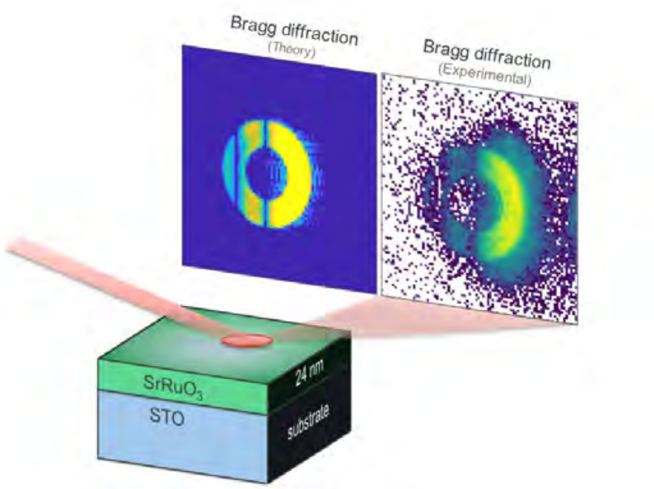


Illustration of Bragg scattering on ferroelectric/ ferromagnetic film stack. The Bragg diffraction is then used to recover information on the intrinsic three-dimensional strain map within the film stack.

Project Description

This research will help to develop techniques critical to understanding how materials structure at the nanometer scale controls its magnetic and electronic behavior. Understanding this critical information is key to unlocking the potential for new magnetic materials that could have broad impact in information systems technology (computers, cell phones, sensors, etc). Understanding how our information systems behave is critical to all aspects of our modern life including commerce and national security.

Technical Outcomes

The project was successful in its development of strain and material imaging techniques on advanced devices via Bragg ptychography. The experimental scope focused on strain imaging on multiferroic films. Strain imaging and nanodiffraction was completed on the device stacks.

Publications

Journal Articles

Carr, A. V., J. M. Bowlan, C. Mazzoli, A. Barbour, W. Hu, S. Wilkins, C. Walker, X. Ding, N. Lee, J. H. Kim, Y. J. Choi, S. Lin, R. L. Sandberg and V. Zapf. Evidence for the Alternating Next-Nearest Neighbor model in the dynamic behavior of a frustrated antiferromagnet. Submitted to *Physical Review Letters*. (LA-UR-20-24289)

Presentation Slides

Carr, A. V., J. M. Bowlan, S. Lin, C. Mazzoli, A. Barbour, W. Hu, S. Wilkens, X. Ding, N. Lee, J. H. Kim, Y. J. Choi, R. L. Sandberg and V. Zapf. Traversing the "Devil's Staircase": Dynamic behavior of a frustrated antiferromagnet. Presented at *NSLS-II Friday Virtual Lunchtime Seminar Series (Webinar)*, Upton, New York, United States, 2020-12-04 - 2020-12-04. (LA-UR-20-29864)

Carr, A. V., V. Zapf, D. A. Yarotski and R. L. Sandberg. LDRD Project Visit: Novel X-ray Imaging to Unlock the Potential of Antiferromagnetic Materials. Presented at *LDRD Project visit*, Los Alamos, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30200)

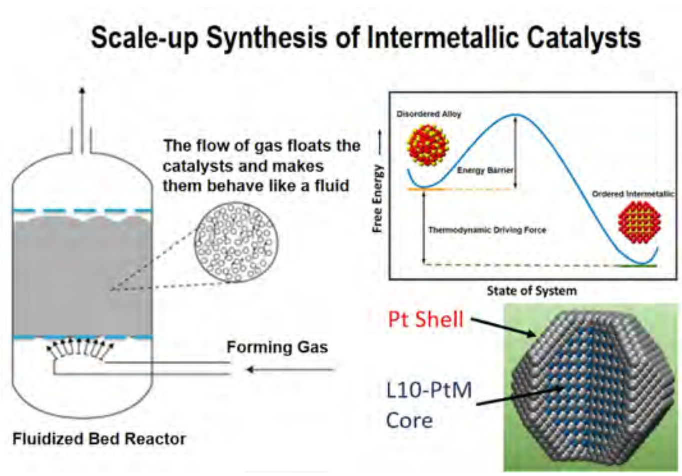
Posters

Burdet, N. G., A. V. Carr, J. M. Bowlan, K. M. Mertes, J. D. Nguyen, R. Tobey, X. Ding, S. Lin, C. S. Walker, B. A. Pound, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins , V. Zapf, C. Mazzoli and R. L. Sandberg. Towards spatially mapping domain dynamics in Antiferromagnetic materials with soft x-ray scattering at NSLS-II. Presented at *SLAC Users Meeting*, Standford, California, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-25092)

**Peer-reviewed*

Synthesis of Platinum-Rare Earth Intermetallic Fuel Cell Catalysts

Jacob Spendelow
20190640PRD3



Understanding how generic parameters of intermetallic catalysts impact their performance/stability in fuel cells is key to fulfilling our tasks proposed in this LDRD project. Without these fundamental conditions, we can not design/synthesize plutonium-rare earth element catalysts with desirable structural features that give arise to optimum fuel cell performance/durability. The project team first developed "fluidized bed reactor" technique to scale up the synthesis, as a large quantity of catalysts can avoid batch-to-batch difference and is essential to a rigorous investigation. Then, the team systematically interrogate the factors (e.g., particle size) and established the correlation between these parameters and fuel cell performance/stability.

Project Description

The project seeks to develop improved fuel cell catalysts. Fuel cells are relevant and important to multiple Department of Energy missions related to energy security, as well as fuel cells for National Nuclear Security Administration-specific national security applications. If successful, we expect that catalysts developed through this project could have transformative impact on fuel cell technology, providing near-term as well as long-term benefits for energy security and national security applications.

Technical Outcomes

The team came up with an innovative method to prepare platinum-rare earth elements catalysts in the ordered intermetallic structures and examined their capabilities in enhancing the efficiency and durability for the hydrogen fuel cell application. The performance improvement in the fuel cell testing is suggestive that more efforts should be spent on further stabilizing the rare earth elements. The goals of the project have been successfully accomplished.

Publications

Journal Articles

Qiao, Z., C. Li, C. Wang, S. Hwang, B. Li, Y. Zeng, A. J. Kropf, C. E. Wegener, Q. Gong, G. Wang, D. Myers, J. Xie, J. S. Spendelow and G. Wu. Synergistic PGM-free Single Metal Sites for Promoting PtCo Ordered Intermetallic Fuel Cell Catalysts: Performance and Durability Improvements. Submitted to *Energy & Environmental Science*. (LA-UR-21-23020)

*Wang, C. and J. S. Spendelow. Recent Developments in Pt-Co catalysts for PEM Fuel Cells. 2021. *Current Opinion in Electrochemistry*. 100715. (LA-UR-20-25517 DOI: 10.1016/j.coelec.2021.100715)

*Zhao, X., C. Xi, R. Zhang, L. Song, C. Wang, J. S. Spendelow, A. I. Frenkel, J. Yang, H. L. Xin and K. Sasaki. High-Performance Nitrogen-Doped Intermetallic PtNi Catalyst for the Oxygen Reduction Reaction. 2020. *ACS Catalysis*. **10** (18): 10637-10645. (LA-UR-20-26461 DOI: 10.1021/acscatal.0c03036)

Presentation Slides

Wang, C. Intermetallic PtCo Catalysts with Enhanced Performance and Stability. . (LA-UR-21-23654)

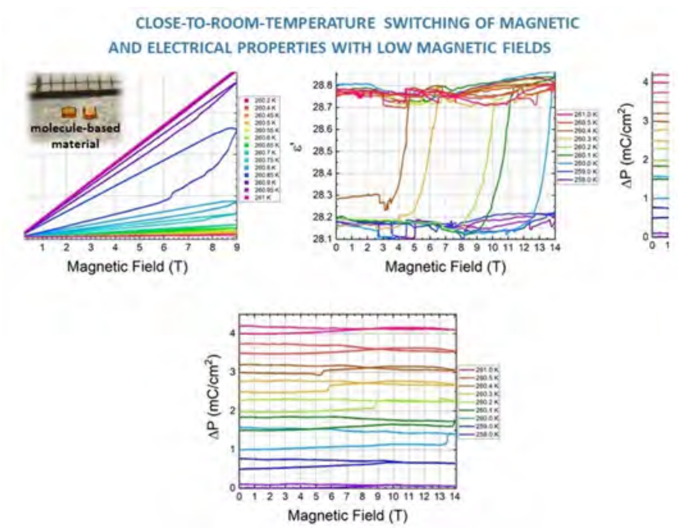
Wang, C., D. Li, Y. S. Kim and J. S. Spendelow. Carbon Effect on the Synthesis and MEA Performances of L10 CoPt Intermetallic Catalysts. Presented at *236th Electrochemical Society Meeting*, Atlanta, Georgia, United States, 2019-10-13 - 2019-10-18. (LA-UR-19-30298)

Wang, C., Z. Qiao, V. B. Kumar, D. A. Cullen, D. Li, K. L. More, G. Wu, Y. S. Kim and J. S. Spendelow. Size-Controlled Synthesis of L10-CoPt Intermetallic Fuel Cell Catalysts on Nitrogen-Doped Mesoporous Graphitized Carbon Support. Presented at *237th Electrochemical Society Meeting*, Montreal, Canada, 2020-05-10 - 2020-05-15. (LA-UR-19-32027)

**Peer-reviewed*

Designing New Ferroelectric Materials with Spin Crossover Transitions

Wanyi Nie
20190647PRD3



A spin crossover phenomenon in molecule-based materials is investigated as a new route to achieving magnetoelectric coupling. In a recent development, the switching of magnetic and electrical properties at an unprecedented high temperature of 261 Kelvin with a record-low magnetic field of 5 Tesla was demonstrated. The discovery is moving this emerging field of research closer to practical applications.

Project Description

The successful demonstration in this project will provide materials for quantum information processing and energy efficient device operation. It will provide new solution for enhancing the information security and energy security missions. Since we are expecting new physical principles in the new material systems, the outcome can lead to high impact results that push the quantum information processing forward under practical operational conditions.

Technical Outcomes

Unprecedentedly, the team achieved magnetoelectric coupling in a molecular spin crossover complex near room temperature and by using a remarkably low magnetic field of 3 Tesla. The project's outcome shows that spin crossovers can be utilized to achieve strong magnetoelectric coupling regardless of the transition temperature opening an avenue for potential applications in classical switching and sensing, and for quantum materials to control, sense and configure the quantum properties of molecular quantum materials.

Publications

Journal Articles

Owczarek, M. T., M. Lee, S. Liu, E. R. Blake, C. S. Taylor, G. A. Newman, J. C. Eckert, J. H. Leal, T. A. Semelsberger, H. Cheng, W. Nie and V. Zapf. Near-Room-Temperature Magnetoelectric Coupling via Spin Crossover in an Iron(II) Complex. 2022. *Angewandte Chemie International Edition*. e202214335. (LA-UR-22-31219 DOI: 10.1002/anie.202214335)

Owczarek, M. T., P. Szklarz and R. Jakubas. Towards ferroelectricity-inducing chains of halogenoantimonates(iii) and halogenobismuthates(iii). 2021. *RSC Advances*. **11** (29): 17574-17586. (LA-UR-20-28039 DOI: 10.1039/D0RA10151F)

*Owczarek, M., M. Lee, V. Zapf, W. Nie and R. Jakubas. Accessing One-Dimensional Chains of Halogenoindates(III) in Organic-Inorganic Hybrids. 2022. *Inorganic Chemistry*. **61** (14): 5469-5473. (LA-UR-22-20744 DOI: 10.1021/acs.inorgchem.2c00374)

Presentation Slides

Owczarek, M. T., M. Lee, W. Nie and V. Zapf. Spin state transitions as a route to magnetoelectric coupling. Presented at *17th International Conference on Molecule Based Magnets*, Manchester, United Kingdom, 2021-06-14 - 2021-06-18. (LA-UR-21-25417)

Owczarek, M. T., M. Lee, W. Nie and V. Zapf. Close-to-room-temperature magnetoelectric coupling in a molecule-based material. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-02-18. (LA-UR-22-21580)

Owczarek, M. T., M. Lee, W. Nie and V. Zapf. Close-to-room-temperature magnetoelectric coupling via spin crossover in Fe(II) molecule-based compound. Presented at *From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information*, Telluride, Colorado, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25338)

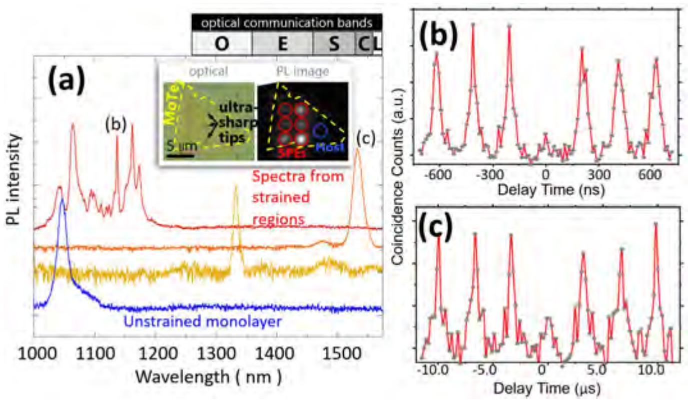
Posters

Owczarek, M. T., M. Lee, J. P. Wampler, W. Nie, V. Zapf, P. Wang, M. Shatruk, J. Eckert, P. Sparks, C. Taylor, E. Blake and G. Newman. Field-induced spin crossover transitions in molecule-based materials. Presented at *EFRC all-hands meeting*, Fort Myers, Florida, United States, 2021-07-09 - 2021-07-11. (LA-UR-21-26303)

**Peer-reviewed*

The Optoelectronic Device Applications of Two-Dimensional Interlayer Moiré Excitons

Han Htoon
20190648PRD3



Quantum light emission at telecommunication wavelength from molybdenum telluride (MoTe2) layers coupled to a nano-pillar arrays. (a) Inset: Optical and photoluminescence image of the sample. Main: Photoluminescence spectra of strained regions (top three traces) show sharp emission of quantum emitters where that of unstrained region (bottom trace) only show emission of two dimensional exciton. (b & c) Hanbury Brwon and Twiss quantum optic experiment performed on the quantum light emission at the position marked in as (b) & (c) in (a) yield clear evidence of single photon emission from two of the quantum emitters emitting at 1160 nm and 1550 nm. This project aims toward developing a new class of ultra-compact and efficient light emitting diodes and has a potential to revolutionize telecommunication, display and flexible electronic industries.

Project Description

Light emitting diodes (LEDs) and lasers lie at the heart of almost all modern technologies. They make high speed internet possible and can be found inside of your television set. This project aims toward developing a new class of ultra-compact and efficient light emitting diodes and lasers by exploiting a novel phenomenon called Moire inter-layer exciton emerged at the interface of two atomically thin semiconductor layers. The devices that could be as thin as 4 atomic layers, can be fabricated by simply stacking different type of atomically thin metallic (graphene) and semiconductor layers in a way similar to Lego blocks. They can also be integrated into existing Silicon-based electronic and photonic integrated circuits. This project therefore has a potential to revolutionize telecommunication, display and flexible electronic industries.

Technical Outcomes

This project established two capabilities essential for deterministic creation of single photon sources in two-dimensional (2D) materials: (1) 2D material layer by layer stacking (2) nanoscale strain engineering capabilities. Utilizing these capabilities, the team demonstrated two novel single photon sources, one based on atomically thin molybdenum ditelluride layers, another based on molybdenum disulfide/tungsten diselenide hetrostructures. These new single photon sources can operate in technologically important near infrared (NIR) spectral range and at liquid nitrogen temperatures.

Publications

Journal Articles

Li, X., A. C. Jones, J. Choi, H. Zhao, V. Chandrasekaran, M. T. Pettes, A. Piryatinski, N. Sinitsyn, S. A. Crooker and H. Htoon. Proximity Induced Chiral Quantum Light Generation in Strain-Engineered WSe2/NiPS3 Heterostructures. Submitted to *Nature Nanotechnology*. (LA-UR-22-20519)

*P. M. T. *. Z. Y. *. H. H. Zhao, H. *., H. Zhao, M. T. Pettes, Y. Zheng and H. Htoon. Site-controlled telecom-wavelength single-photon emitters in atomically-thin MoTe2. 2021. *Nature Communications*. **12** (1): 6753. (LA-UR-21-23958 DOI: 10.1038/s41467-021-27033-w)

Zhao, H., L. Zhu, X. Li, V. Chandrasekaran, J. K. S. Baldwin, M. T. Pettes, A. Piryatinski, L. Yang and H. Htoon. Manipulating Interlayer Excitons for Ultra-pure Quantum Light Generation. Submitted to *Nature Nanotechnology*. (LA-UR-22-23118)

Presentation Slides

Chandrasekaran, V. Quasiparticles in a Nanoscale Correlated Antiferromagnet. Presented at *CINT 2022 Annual Meeting*, Los Alamos, New Mexico, United States, 2022-09-20 - 2022-09-22. (LA-UR-22-29717)

Chandrasekaran, V., D. G. Parobek, A. E. Llacsahuanga Allcca, H. Zhao, X. Li, A. C. Jones, S. A. Ivanov and H. Htoon. Linear polarized photoluminescence from crystalline nanoflakes of NiPS3 antiferromagnet prepared by wet-chemical synthesis. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22376)

Chandrasekaran, V., D. G. Parobek, A. E. Llacsahuanga Allcca, X. Li, H. Zhao, A. C. Jones, S. A. Ivanov and H. Htoon. Confining Many-body Excitons of van der Waals Antiferromagnets to Nanoscale. Presented at *Materials Research Society (MRS) Spring Meeting and Exhibit*, Honolulu, Hawaii, United States, 2022-05-08 - 2022-05-13. (LA-UR-22-29641)

Chandrasekaran, V., M. Titze, A. Flores, A. C. Jones, E. Bielejec and H. Htoon. Ion Implantation and In Situ Optical Characterization for Deterministic Creation of Single Defects. Presented at *MRS Fall 2021*, Boston, Massachusetts, United States, 2021-12-01 - 2021-12-01. (LA-UR-21-31725)

Li, X., A. C. Jones, H. Zhao, V. Chandrasekaran and H. Htoon. Chiral Quantum Light Emitters in 2D Semiconductor/ Magnet Heterostructures. Presented at *APS March Meeting 2022*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-29645)

Li, X., A. C. Jones, H. Zhao, V. Chandrasekaran and H. Htoon. Highly Chiral Quantum Light Emission in 2D Semiconductor/ Magnet Heterostructures. Presented at *2022 MRS Spring Meeting*, Honolulu, Hawaii, United States, 2022-05-08 - 2022-05-13. (LA-UR-22-29643)

Li, X., A. C. Jones and H. Htoon. Magnetic Proximity Effect in TMD/2D-Magnet Heterostructures. Presented at *2021 MRS Fall Meeting*, Boston, Massachusetts, United States, 2021-11-29 - 2021-12-02. (LA-UR-22-29644)

Zhao, H., L. Zhu, M. T. Pettes, X. Li, V. Chandrasekaran, J. K. S. Baldwin, A. Piryatinski, L. Yang and H. Htoon. Near-infrared Quantum Emitters in 2D Semiconductor Heterobilayers. Presented at *MRS Spring Meeting 2022*, Honolulu, Hawaii, United States, 2022-05-09 - 2022-05-09. (LA-UR-22-29123)

Zhao, H., M. T. Pettes, Y. Zheng and H. Htoon. Telecom Quantum Emitters in Atomically-thin MoTe2. Presented at *2021 MRS Fall Meeting*, Boston, Massachusetts, United States, 2021-11-29 - 2021-11-29. (LA-UR-22-29124)

Zhao, H., X. Li, V. Chandrasekaran, M. T. Pettes and H. Htoon. Near-infrared Quantum Emitters in 2D Semiconductor Heterobilayers. Presented at *APS March Meeting 2022*, Chicago, Illinois, United States, 2022-03-16 - 2022-03-16. (LA-UR-22-29122)

Posters

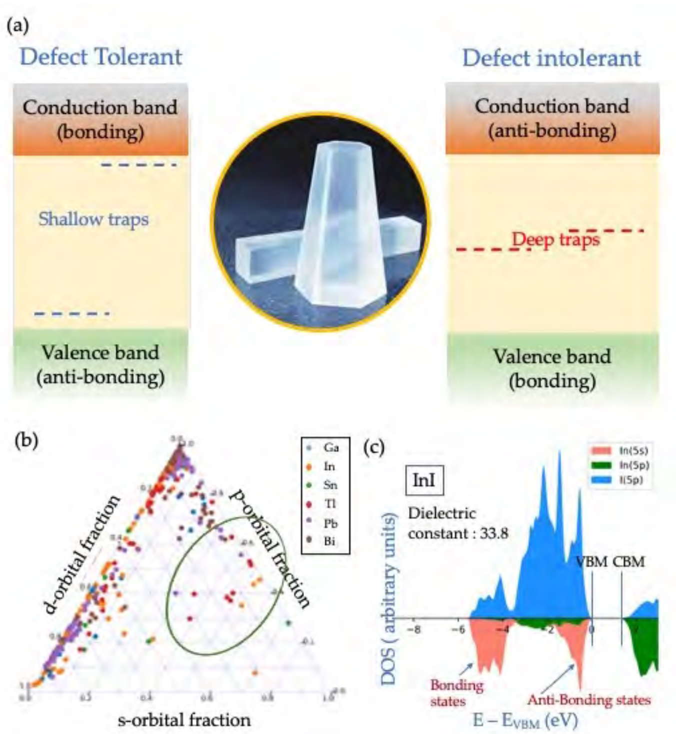
Li, X., A. C. Jones, J. Choi, H. Zhao, V. Chandrasekaran, M. T. Pettes, A. Piryatinski, N. Sinitsyn, S. A. Crooker and H. Htoon. Chiral Quantum Light Emission in 2D Semiconductor/Magnet Heterostructures. Presented at *8th Workshop on Nanotube Optics and Nanospectroscopy (WONTON22)*, Madison, Wisconsin, United States, 2022-07-24 - 2022-07-28. (LA-UR-22-29642)

Zhao, H., L. Zhu, Y. Zheng, X. Li, V. Chandrasekaran, M. T. Pettes, A. Piryatinski and L. Yang. Telecom Quantum Emitters in van der Waals Materials. Presented at *Wonton 2022*, Madison, Wisconsin, United States, 2022-07-25 - 2022-07-29. (LA-UR-22-27428)

**Peer-reviewed*

Defect Tolerant Scintillators: Linking Structure and Performance via Machine Learning (ML)

Anjana Talapatra
20190656PRD4



Signatures of defect tolerant scintillators. (a) Schematic of defect tolerant and intolerant scintillators. Materials with anti-bonding states at the top of the valence band (VBM) and bonding states at the conduction band minimum (CBM), are likely to be defect tolerant and vice versa. (b) Ternary plots demonstrating the partial density-of-states of the VBM for oxide perovskite domain. Materials that contain lone s pairs of electrons (highlighted) on the cation are more likely to exhibit defect tolerance. (c) Sample electronic structure of defect tolerant material (InI). The high energy anti-bonding orbitals appear close to the VBM, signifying defect tolerant behavior.

Project Description

Nuclear processes are associated with the emission of high energy particles capable of ionizing atoms, and detecting this ionization enables the observation of the nuclear process itself and is critical for identifying nuclear materials. One such detection technique is the use of scintillators - materials that convert the energy deposited by incident radiation into visible or ultraviolet photons. However, this irradiation introduces damage in the material, lowering efficiency. This proposal aims to minimize the detrimental effect of defects by tailoring the chemistry of scintillator materials, allowing one to design defect tolerant scintillators that can absorb and nullify the adverse consequences of defects. This will be facilitated via atomistic calculations and machine learning (ML). This work will integrate first-principle calculations, experimental data and ML in line with the Materials Genome Initiative and the laboratory's Science of Signatures and Materials for the Future Science Pillars. Concomitantly, we will develop a fundamental understanding of the relationship between defects and the performance of scintillators which will be applicable to other optical materials as well. New defect-tolerant detector materials will enhance the mission-driven science at both current and future facilities and also impact other arenas such as global security, non-destructive testing and medical imaging.

Technical Outcomes

The project demonstrated the role of defects such as Ruddlesden-Popper phases in scintillator materials and their effect on efficiency of optical materials and achieved an understanding of the relationship between defects and performance. The team identified a large number of defect-tolerant candidates in the ternary chalcogenide and oxide perovskites space using atomistic calculations and Machine Learning paving the way for future proposals to discover mission-relevant optical materials.

Publications

Journal Articles

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. A Machine Learning Approach to Prediction of Formability and Thermodynamic Stability of Single and Double Perovskite Oxides. Submitted to *Chemistry of Materials*. (LA-UR-20-25347)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Band gap predictions of Novel Double Perovskite Oxides using Machine Learning. Submitted to *Chemistry of Materials*. (LA-UR-21-28459)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Supporting Information: Band gap predictions of Novel Double Perovskite Oxides using Machine Learning. Submitted to *Chemistry of Materials*. (LA-UR-21-28478)

*Talapatra, A. A., D. Ghosh, B. P. Uberuaga and G. Pilania. Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. 2021. *Journal of Materials Science*. **56** (28): 15812-15823. (LA-UR-21-23719 DOI: 10.1007/s10853-021-06294-2)

Presentation Slides

Talapatra, A. A. A Machine-Learning based Hierarchical Screening Strategy to Expedite Search of Novel Scintillator Chemistries. Presented at *MRS Fall Meeting, 2019*, Boston, Massachusetts, United States, 2019-12-01 - 2019-12-06. (LA-UR-19-31946)

Talapatra, A. A. A Machine Learning Guided Discovery of Novel Oxide Perovskites for Scintillator Applications. Presented at *TMS 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-22212)

Talapatra, A. A. Accelerating scintillator materials discovery using Machine Learning. . (LA-UR-21-24920)

Talapatra, A. A. A Machine Learning aided hierarchical screening strategy for materials discovery. . (LA-UR-21-27531)

Talapatra, A. A. A Machine-learning Based Hierarchical Framework to Discover Novel Scintillator Chemistries. Presented at *Materials Science & Technology (MS&T 2021)*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-20. (LA-UR-21-30152)

Talapatra, A. A. Introduction to Machine Learning for Materials Scientists. Presented at *Scientific machine learning for materials science applications*, Los Alamos, New Mexico, United States, 2022-08-15 - 2022-08-23. (LA-UR-22-29286)

Uberuaga, B. P. Highlights performed on LANL IC on the project w19_matprops. . (LA-UR-21-24026)

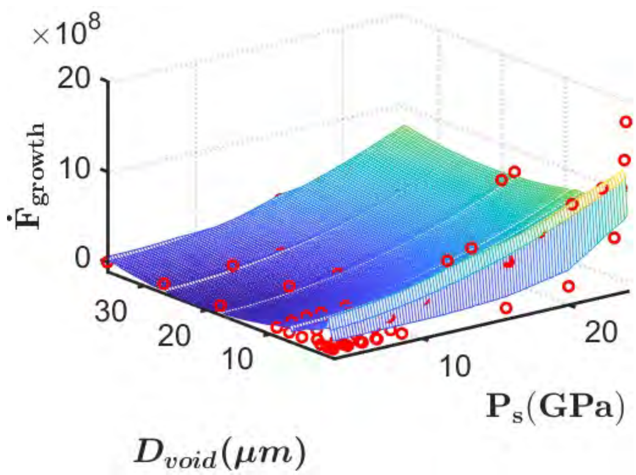
Other

Talapatra, A. A. A Machine Learning aided hierarchical screening strategy for materials discovery. Audio/Visual. (LA-UR-21-27864)

**Peer-reviewed*

Development of Next Generation Microstructure-Aware Burn Models for High Explosives.

Tariq Aslam
20190658PRD4



Microstructure aware reactive burn models are crucial for the controlled design of high explosives (HEs). Traditional reactive burn models implicitly calibrate the relation between the HE microstructure and its sensitivity using expensive experiments. Using LDRD support, the team is developing a machine learning based microstructure aware reactive burn model which is trained using high fidelity reactive meso-scale simulations. The framework informs the fundamental mechanisms through which HEs detonate and explicitly explains the role of microstructural feature on HE sensitivity response, making it a next generation computational tool to tailor HE design for improved safety and performance.

Project Description

The main task is to develop high-fidelity microstructure models to comprehensively understand the physics of energy-localization, reaction initiation and growth at the grain-scale of High Explosives materials. The end goal is to develop a materials-by-design facility that can be used for the design of precisely controlled energy-delivery systems.

Technical Outcomes

The project made tangible progress towards the stated goals. Several items were of importance, namely development of robust computational algorithms needed for chemically reacting compressible flow with non-ideal equations of state, verification of diffusion effects in laminar flames in such flows, and a detailed examination of closure conditions as well as computational infrastructure for such examination.

Publications

Journal Articles

*Rai, N. K. and T. D. Aslam. Evaluation of thermodynamic closure models for partially reacted two-phase mixture of condensed phase explosives. 2022. *Journal of Applied Physics*. **131** (18): 185902. (LA-UR-21-31716 DOI: 10.1063/5.0085208)

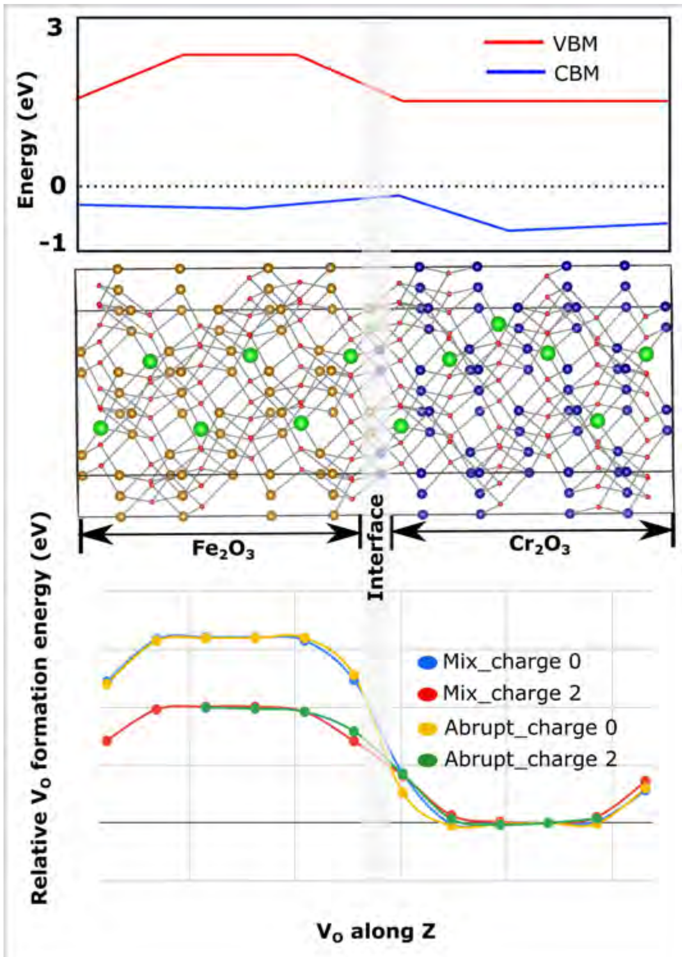
Presentation Slides

Rai, N. K. Next Generation Microstructure-Aware Burn Models for High Explosives. . (LA-UR-21-24186)

**Peer-reviewed*

Importance of Metal/Oxide Interfaces to Design and Tailor Composite Material Properties.

Blas Uberuaga
20200676PRD1



A fundamental understanding of the integrated effects of interfacial complexity with space charge formation, band bending, and species transport under the same level of theory is limited. The present project targets this knowledge gap by elucidating the electronic structure, band bending, defect formation energy, and defect segregation at model interfaces. The figure shows an example of the electronic structure, band bending, and oxygen vacancy formation energy at and near the iron oxide (Fe2O3)/chromium oxide (Cr2O3) interface.

Project Description

Materials are at the heart of energy technologies that have the potential for alleviating many of our current societal challenges, from climate change to energy security. The ability to tune material properties grows exponentially when we can mix materials of two very different natures, such as a metal with an insulating oxide. However, this mixing inevitably leads to interfaces between the two materials, which can have a dramatic impact on the defects that dictate the properties of the material. By examining these interfaces and interrogating the ways in which the interfaces impact defects, we will build a fundamental understanding of this interaction that can then be used in the design of new materials with enhanced functionality for radiation and/or corrosion environments, battery technologies, and catalytic applications. These areas are central to the core mission of Department of Energy.

Technical Outcomes

The primary outcome of this project was examination of the ferric(III) oxide/chromium(III) oxide interface, a model system of more general oxide/oxide interfaces. The project found, using density functional theory, that the interface induced band bending of the electronic structure and that changed the nature of the preferred defects. It also found that the phase structure was a greater sink for defects than the interface itself. These results have implications for damage evolution in composite structures.

Publications

Journal Articles

*Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Critical Assessment of the Thermodynamics of Vacancy Formation in Fe2O3 Using Hybrid Density Functional Theory. 2020. *The Journal of Physical Chemistry C*. **124** (43): 23988-24000. (LA-UR-20-24936 DOI: 10.1021/acs.jpcc.0c07522)

*Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Interplay between defect transport and cation spin frustration in corundum-structured oxides. 2021. *Physical Review Materials*. **5** (3): 034410. (LA-UR-20-28924 DOI: 10.1103/PhysRevMaterials.5.034410)

Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Correction to "Critical Assessment of the Thermodynamics of Vacancy Formation in Fe2O3 Using Hybrid Density Functional Theory". Submitted to *Journal of Physical Chemistry C*. (LA-UR-21-20017)

Yano, K. H., A. A. Kohnert, A. Banerjee, D. J. Edwards, E. F. Holby, T. C. Kaspar, H. Kim, T. G. Lach, S. D. Taylor, Y. Wang, B. P. Uberuaga and D. K. Schreiber. Radiation-Enhanced Anion Transport in Hematite. Submitted to *Chemistry of Materials*. (LA-UR-20-28988)

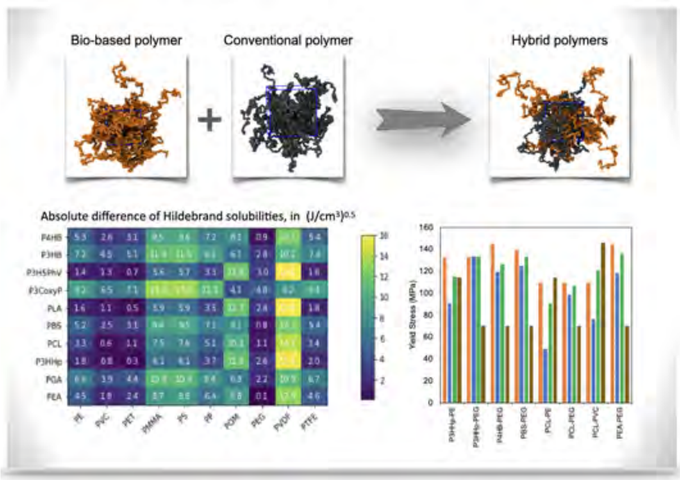
Presentation Slides

Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Interplay between defect transport and cation spin frustration in corundum-structured oxides. Presented at *MRS 2021 Virtual Spring Conference*, Los Alamos, New Mexico, United States, 2021-04-17 - 2021-04-23. (LA-UR-21-24006)

**Peer-reviewed*

Atomistic Modeling and Machine Learning for Bio-Advantaged Polymer Design

Ghanshyam Pilania
20200688PRD2



Funded by an LDRD PRD Fellowship, this project focuses on optimizing degradability-functionality tradeoffs in bio-/conventional hybrid polymer systems using atomistic simulations. The top panel highlights simulated polymers for representative bio-based, conventional and hybrid bio-/conventional polymer chemistries. Starting form a large combinatorial set, a subset of promising polymer chemistries is down-selected based on the relative difference of Hildebrand solubility parameters (HS_diff). For better computability, combinations with low HS_diff in the left panel are selected and their properties are evaluated. As an example, Young's moduli for several binary-copolymers and blends in a 50/50 composition are compared with the corresponding homopolymers (right panel).

Project Description

Plastics are ubiquitous and plastic pollution is currently being considered as one of the largest environment threats. To address this challenge, current research efforts are focused on developing new bio-degradable and bio-compatible polymers which have the potential to replace petroleum-based plastics for a sustainable future. Bio-derived polymers offers a faster degradation; however, they suffer from poor mechanical and elastic properties and high cost of production. To mitigate this shortcoming, this project aims at understanding design rules for improved polymer hybrid materials which combine bio-based chemistries with conventional polymers to achieve the desired favorable combination of functional properties without compromising much on the biodegradability. The main goal of this project is to develop a knowledge base of design rules and to discover, design, and develop new hybrid bio-degradable polymers via combining conventional and bio-advantaged polymers—will enable a more cost-effective, smooth and sustainable path to replace petroleum-based products with sustainable bio-based alternatives. The research is well aligned with the Department of Energy's mission in Clean Energy Innovation. The improved ability to develop eco-friendly bioplastics will lead to a reduced carbon footprint for plastics manufacturing, and innovative solutions to reduce the accumulation and persistence of plastics in the environment.

Technical Outcomes

Molecular dynamics simulations were employed to model a range of hybrid polymers formed via combining a set of bio-based polymers with the most commonly used conventional polymers. Our hierarchical computational screening approach identified eight hybrid copolymer compositions which can be potentially useful for packaging applications and should be considered in future synthesis and testing efforts. Out of these, five are based on polyethylene glycol and exhibit well-established synthesis routes.

Publications

Journal Articles

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Glass Transition Temperature Predictions of Binary Copolymers and Blends of Polyhydroxyalkanoate Biopolymers: Compositional and Configurational Dependence. Submitted to *Macromolecules*. (LA-UR-20-30478)

*Bejagam, K. K., N. S. Gupta, K. Lee, C. N. Iverson, B. L. Marrone and G. Pilania. Predicting the Mechanical Response of Polyhydroxyalkanoate Biopolymers Using Molecular Dynamics Simulations. 2022. *Polymers*. **14** (2): 345. (LA-UR-21-32062 DOI: 10.3390/polym14020345)

Presentation Slides

Bejagam, K. K. In the quest for "Green Polymers". Presented at *CPMU Silver Jubliee meeting*, Bangalore, India, 2020-12-18 - 2020-12-18. (LA-UR-20-30343)

Bejagam, K. K. Atomistic Modeling and Machine Learning for Bio-advantaged Polymer Design. . (LA-UR-21-29152)

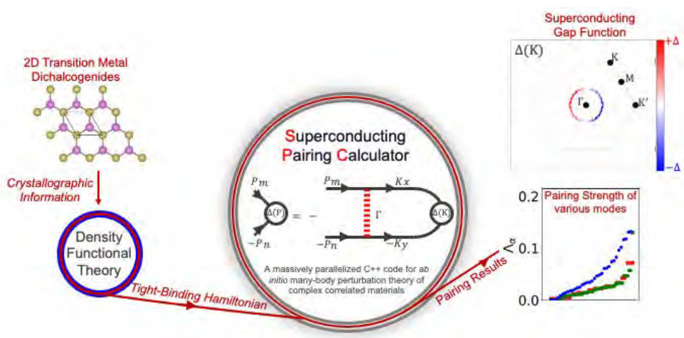
Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Computational aided design of bio-polymers by mining the PHA chemical space. Presented at *ACS spring Meeting 2021*, Los Alamos, New Mexico, United States, 2021-04-05 - 2021-04-16. (LA-UR-21-23600)

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Design of Bio-Polymers by Mining the PHA Chemical Space. Presented at *International Conference on Biopolymers and Bioplastics*, Los Alamos, New Mexico, United States, 2021-06-21 - 2021-06-22. (LA-UR-21-26177)

**Peer-reviewed*

Topological Superconductivity in Van der Waals Materials as a Platform for Qubits

Christopher Lane
20200756PRD3



Theoretical insights into superconducting pairing are typically limited to toy-models designed to extract specific physical properties for a general class of materials. In response, LDRD supported researchers at Los Alamos have developed a new advanced theoretical capability to make robust predictions in material specific detail. By building on accurate density functional theory derived Hamiltonians, the new code directly calculates superconducting instabilities and gap functions in an efficient massively parallel manner. With this new tool in hand, the team aims to hopefully predict topological superconductivity in the two-dimensional transition metal dichalcogenides as a platform for a new generation of qubits.

Project Description

In December 2018, the National Quantum Initiative (NQI) Act was signed into law to speed up the advancement of quantum related technology and quantum computing. The Department of Energy is expected to invest heavily in materials science for quantum information processing in the next five years, including the National Quantum Information Science Research Centers. By performing simulations based on the coherent superposition of quantum states, quantum computers hold huge promise to transform our society by solving tough problems intractable on our classical computers built with on-off bit technology. The grand challenge facing the quantum computers is the overhead from the error correction needed to combat the decoherence. Therefore, quantum bits with long coherence time are desirable. This project directly addresses this challenge by searching and identifying the topological superconductivity in two-dimensional transition-metal dichalcogenides and their heterostructures. Topological superconductors are believed to host the exotic quasiparticles, the so called Majorana fermion modes. The quantum bits built upon these exotic particles will enable fault-tolerant quantum computation that is immune to conventional decoherence sources. Success from this project will provide a fundamental understanding and design principles of topological superconductivity, paving the way for robust quantum information platforms.

Technical Outcomes

This project has successfully identified topological superconductivity in the two-dimensional transition-metal dichalcogenides. The goal of this project was successfully achieved by developing a new theoretical capability to identify topological superconductivity material specific detail. During the course of this project the team also examined signatures of possible unconventional superconductivity in other material families in collaboration with world class experimental and theoretical groups. Both of these efforts significantly advanced our understanding of quantum materials.

Publications

Journal Articles

*Ghosh, S., C. Lane, F. Ronning, E. D. Bauer, J. D. Thompson, J. -. Zhu, P. F. S. Rosa and S. M. Thomas. Colossal piezoresistance in narrow-gap Eu5In2Sb6. 2022. *Physical Review B*. **106** (4): 045110. (LA-UR-21-26019 DOI: 10.1103/PhysRevB.106.045110)

Hu, Y., C. A. Lane, X. chen, S. Peng, Z. Sun, M. Hashimoto, D. Lu, T. Wu, R. S. Markiewicz, X. Chen, A. Bansil, s. wilson and J. He. A unified route towards nodal metallicity in doped spin-1/2 antiferromagnetic Mott insulators. Submitted to *Science*. (LA-UR-22-32240)

Huang, Z., C. A. Lane, D. A. Yarotski, A. J. Taylor and J. Zhu. Topological superconducting domain walls in magnetic Weyl semimetals. Submitted to *Physical Review Letters*. (LA-UR-21-25206)

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*Lane, C. and J. Zhu. Identifying topological superconductivity in two-dimensional transition-metal dichalcogenides. 2022. *Physical Review Materials*. **6** (9): 094001. (LA-UR-22-23485 DOI: 10.1103/PhysRevMaterials.6.094001)

Markiewicz, R. S., B. Singh, C. A. Lane and A. Bansil. High-order Van Hove singularities in cuprates and related high-Tc superconductors. Submitted to *Nature Communications*. (LA-UR-21-22462)

*Matt, C. E., Y. Liu, H. Pirie, N. C. Drucker, N. H. Jo, B. Kuthanazhi, Z. Huang, C. Lane, J. Zhu, P. C. Canfield and J. E. Hoffman. Spin-polarized imaging of strongly interacting fermions in the ferrimagnetic state of the Weyl candidate CeBi. 2022. *Physical Review B*. **105** (8): 085134. (LA-UR-20-28429 DOI: 10.1103/PhysRevB.105.085134)

*Peng, S., C. Lane, Y. Hu, M. Guo, X. Chen, Z. Sun, M. Hashimoto, D. Lu, Z. Shen, T. Wu, X. Chen, R. S. Markiewicz, Y. Wang, A. Bansil, S. D. Wilson and J. He. Electronic nature of the pseudogap in electron-doped Sr2IrO4. 2022. *npj Quantum Materials*. **7** (1): 58. (LA-UR-20-26487 DOI: 10.1038/s41535-022-00467-1)

Setty, C., C. A. Lane, L. Chen, H. Hu, J. Zhu and Q. Si. Electron correlations and charge density wave in the topological kagome metal FeGe. Submitted to *Physical Review Letters*. (LA-UR-22-21964)

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Zhang, R., C. A. Lane, B. Singh, J. Nokelainen, B. Barbiellini, R. S. Markiewicz, A. Bansil and J. Sun. f-electron and magnetic ordering effects in nickelates LaNiO2 and NdNiO2: remarkable role of the cuprate-like 3dx2−y2 band. Submitted to *npj Quantum Materials*. (LA-UR-20-27054)

Zhang, R., C. A. Lane, J. Nokelainen, B. Singh, B. Barbiellini, R. S. Markiewicz, A. Bansil and J. Sun. Fingerprints of nematicity and competing orders in the infinite-layer nickelate. Submitted to *Physical Review X*. (LA-UR-22-25386)

Zhang, R., C. A. Lane, J. Nokelainen, B. Singh, B. Barbiellini, R. S. Markiewicz, A. Bansil and J. Sun. Fingerprints of nematicity and competing orders in the infinite-layer nickelate. Submitted to *Physical Review X*. (LA-UR-22-25838)

Presentation Slides

Lane, C. A. and J. Zhu. Identifying Topological Superconductivity in the 2D Transition Metal Dichalcogenides. Presented at *APS March Meeting 2021*, los alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22432)

Matzelle, M., C. A. Lane, R. He, R. S. Markiewicz and A. Bansil. An ab initio Study of Oxygen Vacancies in Ba2CuO3+\xce \xb4. Presented at *APS March Meeting 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22472)

Ning, J., C. A. Lane, M. Matzelle, B. Singh, B. Barbiellini, R. S. Markiewicz, A. Bansil and J. Sun. Accurate lattice dynamics of cuprates from first principles. Presented at *APS March Meeting 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22479)

Zhu, J. Dark Matter Detection with Strongly Correlated Topological Matter: Flatband Effect. Presented at *Quantum Matter & Beyond*, Jacksonville Beach, Florida, United States, 2021-12-15 - 2021-12-17. (LA-UR-21-32248)

Zhu, J. Dark Matter Detection with Strongly Correlated Topological Matter: Flatband Effect. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21944)

Zhu, J. and C. A. Lane. Density functional theory (DFT): A Primer. . (LA-UR-21-30165)

Zhu, J. and C. A. Lane. Density Functional Theory (DFT): Practical Implementation and Numerical Convergence. . (LA-UR-22-26783)

Zhu, J. and C. A. Lane. Density Functional Theory (DFT): Electronic Structure. . (LA-UR-22-27482)

Posters

Lane, C. A. and J. Zhu. Chiral Topological Superconductivity in Prototypical 2D Transition-Metal Dichalcogenides. Presented at *CECAM Flagship Workshop: Green's function methods: the next generation 5*, Toulouse, France, 2022-11-15 - 2022-11-18. (LA-UR-22-31626)

**Peer-reviewed*

Synthesis and Stabilization of Two-Dimensional Electrenes as Novel Nanoscale Magnets

Sergei Ivanov
20200776PRD4

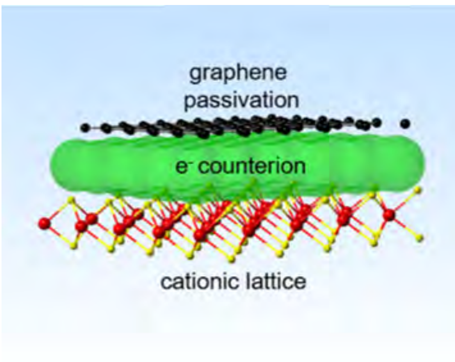


Figure 1: Electrenes are two-dimensional (2D) ionic crystals with an exotic structure consisting of a cationic sub lattice and electron counterion that can be passivated with graphene, creating a 2D architecture for nanoscale devices. The National Quantum Initiative has identified 2D materials as a key platform to realize quantum information science & technology; both the range of accessible material properties and the 2D nature of electrenes make this system an important, yet relatively unexplored, 'building block' for quantum information, science and technology (QIS&T) material where Los Alamos National Laboratory could take the lead.

Project Description

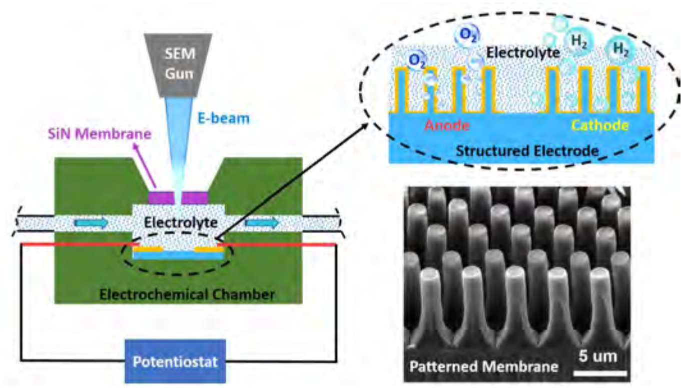
Electrides are ionic crystals wherein unbound electrons act as anions filling voids between inorganic cations in the crystal structure. The differing dimensionality of the void space results in varying electronic or magnetic properties, which is further expanded when approaching the nanoscale. When electrides are prepared as two-dimensional (2D) nanosheets, i.e. electrenes, the unbound electron is still retained having potential uses in spintronic, negative refractive index, and superconductor applications. This project aims to develop new synthetic protocols for electride materials to avoid the use of solid state reactions which are energy and time intensive. The success of this endeavor will result in a streamlined methodology that will result in the easy access of this exotic material for the study and development of its properties for its eventual use in quantum science. The National Quantum Initiative (of which the Department of Energy is an "integral partner") has identified 2D materials as a key platform to realize quantum information science & technology; both the range of accessible material properties and the 2D nature of electrenes make this system an important, yet relatively unexplored, 'building block' quantum information, science and technology (QIS&T) material where Los Alamos National Laboratory could take the lead.

Technical Outcomes

The goal of the project was to develop new synthetic protocols for electride materials to remove the dependence on solid state methodologies. The team was capable of synthesizing the electride through solid state methodologies Progress was made on the project to determine root causes of deficiency arising from product oxidation before it could be isolated from the reactant solution.

Multi-Scale Visualization for Tuning High-Efficiency and Low-Catalyst-Loading

Ulises Martinez
20200777PRD4



A new operando electron-microscopy-based characterization technique is being developed to visualize water splitting reactions at nano- and micro-scales to aid in the design of new electrode structures for improved performance of polymer electrolyte membrane electrolyzer cells (PEMECs). This new technique will bridge the gap between three electrode systems for materials development and PEMEC devices used for performance evaluation. Fundamental understanding gained will allow development of next-generation structured electrodes with increased catalyst utilization and decreased precious metal content, increasing performance, while at the same time, decreasing costs of electrochemical energy conversion and storage devices. [Image credit: Los Alamos National Laboratory]

Project Description

This projects seeks to develop a new Los Alamos National Laboratory capability which will directly impact the design and development of new electrode structures for electrochemical energy storage and conversion devices such as electrolyzers and fuel cells. Electrolyzers and fuel cells are relevant and important to multiple Department of Energy (DOE) missions related to energy security, including DOE's Earthshots Initiative. Successful development of this novel technique will be transformative, significantly impacting the design of new electrode structures for energy-related electrochemical devices with improved performance and durability, providing near-term as well as long-term benefits for energy security and national security applications.

Technical Outcomes

The overall goal of this project was to develop an operando visualization technique for the study of water splitting mechanisms for polymer electrolyte membrane electrolyzer cells. The team was able to successfully combine electron microscopy and micro-fabrication techniques such as e-beam deposition and focused ion beam to develop a new capability to study novel electrode materials for clean-energy applications such as electrolyzers and fuel cells, allowing to with challenges associated with intermittent renewable energy sources.

Publications

Journal Articles

Yang, G., C. H. Lee, X. Qiao, S. Komini Babu, U. Martinez and J. S. Spendelow. Advanced Electrode Structures for Proton Exchange Membrane Fuel Cells: Current Status and Path Forward. Submitted to *Advanced Materials*. (LA-UR-22-23045)

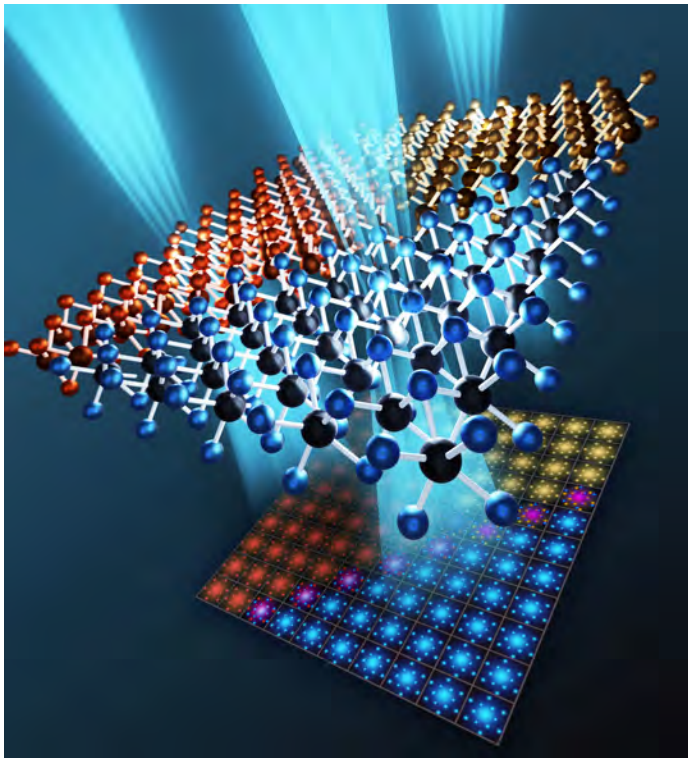
Presentation Slides

Yang, G. Structured Membrane-electrode Interface for Highly Efficient PEM Fuel Cell. . (LA-UR-21-22645)

**Peer-reviewed*

Coupling Multiple Patterned Electron Probes for Real Time Orientation, Lattice Parameter, and Strain Mapping at the Nanoscale

Michael Pettes
20220485MFR



Overall concept of the capability developed in this project illustrating the concept of four-dimensional scanning transmission electron microscopy (artwork: Sarah Tasseff, LANL).

Project Description

Modern fast electron detectors have been in use for nearly 10 years, with one recently installed on our new probe-corrected transmission electron microscope. Problems common to all big data characterization methods have precluded the practical use of these new detectors for the innovative new capabilities that they can offer, especially related to areas that benefit from large datasets including machine-learning. Our project will solve this roadblock by delivering an uncertainty-based four-dimensional scanning transmission electron microscopy (4D-STEM) capability to the Plutonium Center of Excellence at Los Alamos National Laboratory which will enable real-time data analyses of crystallographic orientation and strain at the nanoscale to understand key fundamental science questions in actinide (Plutonium and Uranium) research. Most promising, our phase 2 goal will produce a machine-learning-based orientation analysis code – including uncertainty quantification – integrated directly with a new multi-beam electron diffraction (MBED) data acquisition capability. This project will lead to the first automated crystal orientation mapping (ACOM) software package integrated into the 4D-STEM data acquisition system at Los Alamos Technical Area-55 for real time extraction of three-dimensional (3D) structural properties including, the holy grail "orientation + phase" descriptor that has to date been unobtainable in standard transmission electron microscope practice.

Publications

Journal Articles

Saxena, A. B., C. Perez-Junyent, M. Porta, E. Valdez, L. Manosa, A. Planes and E. Vives. Flexocaloric effect in superelastic materials. Submitted to *Applied Physics Reviews*. (LA-UR-22-30086)

Saxena, A. B., M. Porta, T. Castan and A. Planes. Caloric effects induced by uniform and non-uniform stress in shape-memory materials. Submitted to *Shape Memory and Superelasticity*. (LA-UR-22-32246)

Presentation Slides

Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials. Presented at *Invited Seminar at Texas A&M University, Department of Materials Science and Engineering*, College Station, Texas, United States, 2022-08-29 - 2022-08-29. (LA-UR-22-28999)

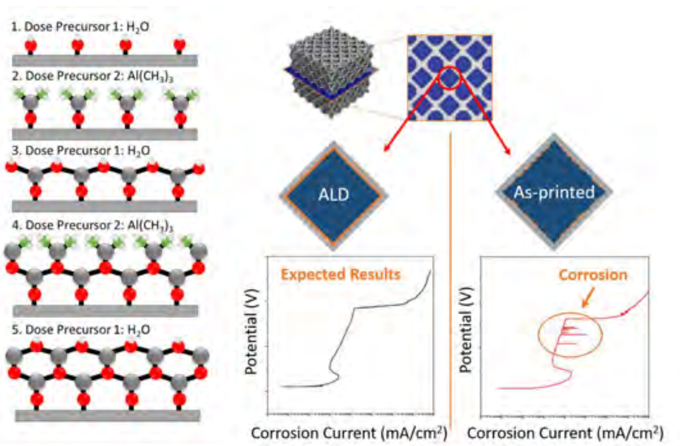
Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials. Presented at *Invited Seminar at University of Virginia, Department of Mechanical and Aerospace Engineering*, Charlottesville, Virginia, United States, 2022-09-15 - 2022-09-15. (LA-UR-22-29469)

Pettes, M. T. Defect and Strain Engineering: Advanced Characterization at the Nanoscale. Presented at *Invited seminar to the LANL BLABS Series*, Los Alamos, New Mexico, United States, 2023-01-23 - 2023-01-23. (LA-UR-23-20663)

**Peer-reviewed*

Tailoring Corrosion Resistance of Additively Manufactured Metals with Atomic Layer Deposition

Timothy Gorey
20220505MFR



As indicated by corrosion current spikes (right graph), as-printed additively manufactured stainless steel has high corrosion susceptibility due to reactive nucleation sites formed in the print process. Using gas intrusion atomic layer deposition of alumina (left), uniform, atomic layers can be deposited onto complex geometry, 3D-printed metal parts with internal surfaces. Steps 4 and 5 of the deposition process can be repeated up to the desired film thickness. These coatings are expected to have highly improved corrosion resistance and part reliability (left graph).

Project Description

As three-dimensional (3D)-printed metals become increasingly integrated with weapon systems, there is an urgent need for finishing techniques that can improve reliability and interchangeability with legacy parts. This integration of 3D-printed components is presently hindered by poor corrosion behavior compared to traditionally manufactured parts. Atomic Layer Deposition (ALD) of thin film, corrosion-resistant barriers offers a clear path to fulfilling this need. In ALD, sequential deposition of individual atomic layers up to a desired thickness offers the ability to coat 3D-printed parts of complex geometry with high conformity. ALD provides a universal solution, where almost any material can be given almost any coating with atomic precision. This positions ALD at the forefront of finishing strategies for 3D-printed components. Overcoming corrosion susceptibility will expand the application of 3D-printed metals across National Security applications and provide meaningful impact to the scientific community by extending the reliability of these metals.

Publications

Reports

Gorey, T. J. Tailoring Corrosion Resistance of Additively Manufactured Metals with Atomic Layer Deposition. Unpublished report. (LA-UR-22-23433)

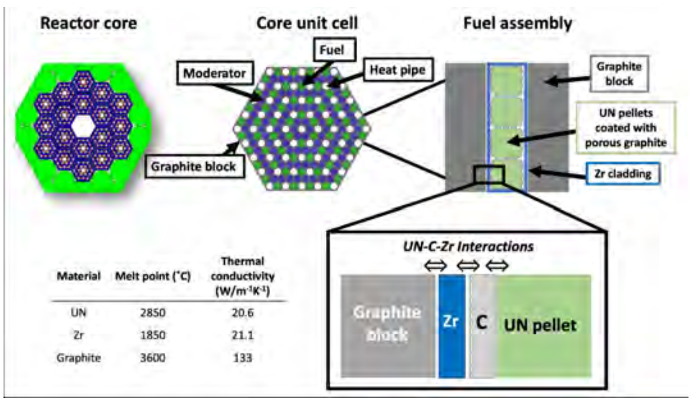
Presentation Slides

Gorey, T. J., D. J. Safarik, I. O. Usov, R. Jones and M. G. Heidlage. Ultra-thin, Conformal ALD Films for Reliable Corrosion Resistance in SLM Metal Additive Manufactured Surfaces. Presented at *American Vacuum Society (AVS) International Symposium and Exhibition*, Pittsburgh, Pennsylvania, United States, 2022-11-06 - 2022-11-11. (LA-UR-22-31644)

**Peer-reviewed*

Interfaces that Enable Advanced Fuels for Enhanced Microreactor Performance

Erofili Kardoulaki
20220506MFR



Schematic of the microreactor core, core unit cell, proposed fuel assembly, and enlarger cross section of the fuel/coating/cladding/core block interface along with key properties for the proposed materials. Understanding and controlling the interfaces between the different constituents of the fuel/cladding assembly is crucial for enhanced performance and will be the focus of the project.

Project Description

Multiple United States agencies are investing in microreactor technologies to support electricity needs in remote locations, disaster relief zones, or remote military bases. Los Alamos National Laboratory (LANL) is a key partner with industry and multiple government organizations who are currently designing and planning to deploy microreactors. For LANL to support these programs and lead its partners to success, efficient microreactor designs that depend on appropriate materials solutions are advocated. LANL's designs rely on materials and fuel-cladding assemblies that can provide high thermal conductivity throughout the reactor's lifetime, withstand off-normal operation, and retain gaseous fission products to increase safety margins. Here, we propose a system comprised of monolithic uranium nitride (UN) pellets, coated with a porous graphite buffer layer, and clad in zirconium (Zr). This multilayered system has the potential to enable efficient microreactor performance by increasing the operating temperature (currently typically below 800 °C), enhancing safety margins, and maximizing fissile mass for fuel longevity. Phase 1 of this proposal will establish the potential of the proposed fuel-cladding system by assessing the high temperature (800-1400 °C) reactions between its constituents and the effect any reactions have on the overall system thermal transport and mechanical properties of the cladding.

Publications

Journal Articles

Kardoulaki, E., N. M. Abdul-Jabbar, D. D. Byler, M. M. Hassan, S. C. Mann, T. P. Coons and J. T. White. Carburization Kinetics of Zircalloy-4 and Its Implication for Small Modular Reactor Performance. 2022. *Materials*. **15** (22): 8008. (LA-UR-22-27783 DOI: 10.3390/ma15228008)

Presentation Slides

Kardoulaki, E. Nuclear fuels and interfaces for advanced specialty reactors. Presented at *MST-8 talk*, Los Alamos, New Mexico, United States, 2022-04-05 - 2022-04-05. (LA-UR-22-23106)

Kardoulaki, E. Interfaces that Enable Advanced Fuels for Enhanced Microreactor Performance. Presented at *NPF Capability review lightning talk*, Los Alamos, New Mexico, United States, 2023-03-13 - 2023-03-13. (LA-UR-23-22505)

Kardoulaki, E. Nuclear fuels and interfaces for advanced specialty reactors. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-23. (LA-UR-23-22761)

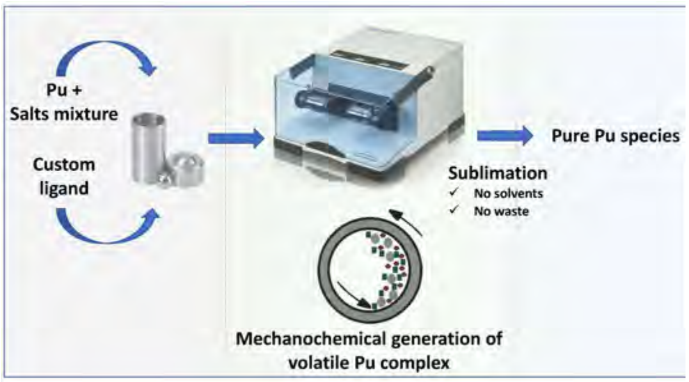
Posters

Kardoulaki, E., N. M. Abdul-Jabbar, D. D. Byler, S. C. Mann, J. T. White and K. J. Mcclellan. Interfaces that Enable Advanced Fuels for Enhanced Microreactor Performance. Presented at *NPF Capability review*, Los Alamos, New Mexico, United States, 2023-04-25 - 2023-04-25. (LA-UR-23-22506)

**Peer-reviewed*

Mechanochemical, Solventless Separation of Plutonium from Chloride Salt Residues

Tatyana Elkin
20220518MFR



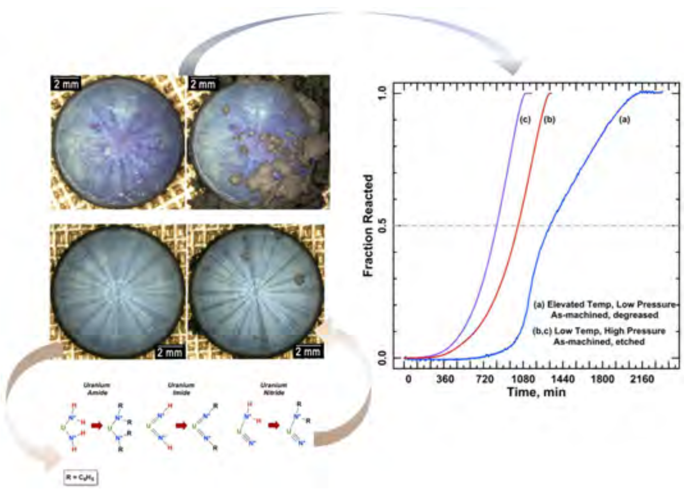
The volatile metal complexes are formed when a Pu-containing mixture is mixed together with an appropriate ligand that is developed in collaboration between LANL and University of Illinois Urbana-Champaign. Because of the big gap between the sublimation temperatures of Pu complexes and the remaining salts, only the Pu species are then sublimed out of the mixture, leading to solventless, and as a result, wasteless separation of Pu from the production mixture.

Project Description

Current methods for plutonium (Pu) chloride salt separations employ large amounts of acid and the organic solvent. Typical processes involve tens of liters of solvent and kilograms of salt, resulting in high volumes of feed to the current aqueous purification process. In fact, significant volumes of waste associated with Pu production dating back to the Manhattan Project that are currently stored in facilities such as the Hanford Site and the Savannah River Site continue to be a major concern for the United States. More recently, waste disposition has also been identified as one of the limiting factors to achieving the needed number of pits per year Pu manufacturing mission. Our mechanochemical approach would significantly decrease the amount of waste produced from the process by enabling a simple process for recovering Pu from the salt residues, which could then be used as a concentrated feed to the aqueous purification process.The development of such strategies to minimize or eliminate waste is a key to furthering actinide science in the coming decades.

Rust, Dust, and a Passive Future-Resilient Actinide Materials

Samantha Lawrence
20200481MFR



Elucidating mechanisms and kinetics of hydride corrosion of uranium is critical for predicting and controlling material degradation during service in complex environments. LANL researchers are applying a combination of solution chemistry and gas-solid techniques to understand the chemical reactions that take place between uranium metal and other molecular species, which drive fundamental hydride corrosion mechanisms and dictate hydride reaction kinetics.

Project Description

Despite years of research, unanswered fundamental questions persist surrounding the causes of uranium corrosion in hydrogen-containing environments. This project aims to understand the chemical reactions that take place at uranium metal surfaces that ultimately dictate corrosion rates. This will be accomplished by studying, for the first time, complimentary solution and gas-solid chemical reactions that occur under hydrogen-containing environments with uranium. The data obtained from this work will inform physics and chemistry-based models of uranium corrosion, which will ultimately enhance our predictive capability.

Technical Outcomes

The solution chemistry experiments executed during this project resulted in the discovery of a new class of uranium complexes. The project also established and improved several hydrogen reaction capabilities, including the ability to conduct uranium-hydrogen reaction experiments at neutron and synchrotron x-ray beam line facilities. The novel data collected during this project are contributing to better understanding of the complex interactions between uranium and hydrogen-containing environments.

Publications

Presentation Slides

Lawrence, S. K. Studying Hydrogen-Metal Interactions at the Lujan Center. Presented at *Informal team meeting*, Online, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21879)

Lawrence, S. K. The Lighter Side of Heavy Metals: Science at the Frontier of Uranium Metallurgy. Presented at *Stewardship Science Graduate Fellowship Annual Program Review*, Santa Fe, New Mexico, United States, 2022-06-21 - 2022-06-23. (LA-UR-22-25601)

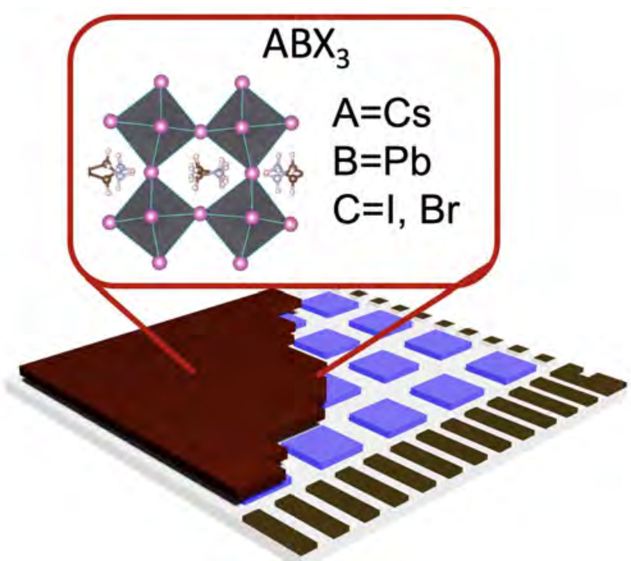
Lawrence, S. K. The Lighter Side of Heavy Metals. Presented at *Department Seminar at Colorado School of Mines*, Golden, Colorado, United States, 2023-03-16 - 2023-03-16. (LA-UR-23-22449)

Lawrence, S. K. and D. T. Carver. In-situ hydriding of depleted uranium: A search for preferential nucleation sites. Presented at *NSLS-II & CFN Joint Users' Meeting*, Virtual, New York, United States, 2021-05-17 - 2021-05-20. (LA-UR-21-24890)

**Peer-reviewed*

Solution Fabricated Solid-State X-ray Imager

Wanyi Nie
20210533MFR



Schematic illustration of the concept of this project. Specifically, we propose to fabricate metal halide perovskite semiconductor layer on pixelated electrodes by solution method. The perovskite material explored here follows a general chemical formula of ABX3, where A is cation, B is Pb and C refers to halide (i.e., I, Br). This device will be tested for X-ray imaging performances, where the perovskite layer will convert X-ray photon into electrical signal that can be collected by the electrodes.

Project Description

X-ray imaging is a non-destructive tool that is widely used in advanced accelerators facility, nuclear material manufacturing and other material science applications. It requires highly sensitive detectors to image the X-ray signal. Semiconductor based X-ray imager that directly converts X-ray photon to electrical signal provides the best conversion efficiency among other technologies in ideal case. However, the current state-of-the-art technology uses amorphous selenium as X-ray absorber that suffers from poor charge extraction efficiency and high fabrication costs that undermines their wide use. We propose to fill the gap with demonstrating new semiconductor-based X-ray imager. Here, we will investigate lead-halide perovskite semiconductor, a solution processable material, for high resolution X-ray imager applications. Leveraging our previous breakthrough in high efficiency perovskite X-ray detector demonstration, we expect to build large scale imagers with high performances. The successful demonstration will provide new route for cost-effective X-ray imager fabrication with high sensitivity and spatial resolutions

Technical Outcomes

The team successfully demonstrated a new high throughput, printable method to build high efficiency X-ray sensing devices. This included the technical achievement of a new “high-throughput”, high-quality crystalline layer fabrication method, and the development and testing of a new high-efficiency, high-resolution perovskite detector. The project’s achievements are intellectual property and high-impact publications, including the designation of one of the “top-10 achievements of 2020” by Physics World.

Publications

Journal Articles

Anirudh, R., R. Archibald, M. S. Asif, M. M. Becker, S. Benkadda, P. Bremer, R. H. S. Bude, C. S. Chang, L. Chen, R. M. Churchill, J. Citrin, J. A. Gaffney, A. Gainaru, W. Gekelman, T. Gibbs, S. Hamaguchi, C. Hill, K. Humbird, S. Jalas, S. Kawaguchi, G. Kim, M. Kirchen, S. Klasky, J. L. Kline, K. Krushelnick, B. Kustowski, G. Lapenta, W. Li, T. Ma, N. J. Mason, A. Mesbah, C. Michoski, T. Munson, I. Murakami, H. N. Najm, K. E. J. Olofsson, S. Park, J. L. Peterson, M. Probst, D. Pugmire, B. Sammuli, K. Sawlani, A. Scheinker, D. P. Schissel, R. J. Shalloo, J. Shinagawa, J. Seong, B. K. Spears, J. Tennyson, J. Thiagarajan, C. M. Ticos, J. Trieschmann, J. van Dijk, B. Van Essen, P. Ventzek, H. Wang, J. T. L. Wang, Z. Wang, K. Wende, X. Xu, H. Yamada, T. Yokoyama and X. Zhang. 2022 Review of Data-Driven Plasma Science. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-22-24834)

I. Falato, M. J., B. T. Wolfe, N. T. T. Nguyen-Fotiadis, X. Zhang and Z. Wang. Contour Extraction of ICF Images With Deep Learning. Submitted to *Review of Scientific Instruments*. (LA-UR-22-24951)

*Kobbekaduwa, K., S. Shrestha, P. Adhikari, E. Liu, L. Coleman, J. Zhang, Y. Shi, Y. Zhou, Y. Bekenstein, F. Yan, A. M. Rao, H. Tsai, M. C. Beard, W. Nie and J. Gao. In-situ observation of trapped carriers in organic metal halide perovskite films with ultra-fast temporal and ultra-high energetic resolutions. 2021. *Nature Communications*. **12** (1): 1636. (LA-UR-20-27180 DOI: 10.1038/s41467-021-21946-2)

Liu, F., R. Wu, J. Wei, W. Nie, A. D. Mohite and S. Brovelli. Recent Progress in Halide Perovskite Radiation Detectors for Gamma-Ray Spectroscopy. Submitted to *ACS Energy Letters*. (LA-UR-22-22600)

*Pan, L., S. Shrestha, N. Taylor, W. Nie and L. R. Cao. Determination of X-ray detection limit and applications in perovskite X-ray detectors. 2021. *Nature Communications*. **12** (1): 5258. (LA-UR-21-28788 DOI: 10.1038/s41467-021-25648-7)

Shrestha, S., H. Tsai and W. Nie. A perspective on the device physics of lead halide perovskite semiconducting detector for Gamma and X-ray sensing. Submitted to *Applied Physics Letters*. (LA-UR-22-33203)

Shrestha, S., X. Li, H. Tsai, C. Hou, H. Huang, D. Ghosh, J. Shyue, L. Wang, S. Tretiak, X. Ma and W. Nie. Long carrier diffusion length in two-dimensional lead halide perovskite single crystals. Submitted to *CHEM*. (LA-UR-21-29516)

Tsai, H., D. Ghosh, W. Panaccione, L. Su, C. Hou, L. Wang, L. R. Cao, S. Tretiak and W. Nie. Addressing the voltage induced instability problem of perovskite semiconductor detectors. Submitted to *ACS Energy Letters*. (LA-UR-22-30015)

*Tsai, H., H. Huang, J. Watt, C. Hou, J. Strzalka, J. Shyue, L. Wang and W. Nie. Cesium Lead Halide Perovskite Nanocrystals Assembled in Metal-Organic Frameworks for Stable Blue Light Emitting Diodes. 2022. *Advanced Science*. **9** (14): 2105850. (LA-UR-21-30401 DOI: 10.1002/advs.202105850)

*Tsai, H., S. Shrestha, L. Pan, H. Huang, J. Strzalka, D. Williams, L. Wang, L. R. Cao and W. Nie. Quasi-2D Perovskite Crystalline Layers for Printable Direct Conversion X-Ray Imaging. 2022. *Advanced Materials*. **34** (13): 2106498. (LA-UR-21-29520 DOI: 10.1002/adma.202106498)

Wang, Z., C. Dujardin, M. S. Freeman, A. E. Gehring, J. F. Hunter, P. Lecoq, W. Liu, C. L. Melcher, C. Morris, M. Nikl, G. Pilania, R. Pokharel, D. G. Robertson, D. J. Rutstrom, S. K. Sjue, A. S. Tremsin, S. A. Watson, B. W. Wiggins, N. M. Winch and M. Zhuravleva. Needs, trends, and advances in scintillators for radiographic imaging and tomography. Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-22-32994)

Wolfe, B. T., M. J. I. Falato, X. Zhang, N. T. T. Nguyen-Fotiadis, J. P. Sauppe, P. M. Kozlowski, P. A. Keiter, R. E. Reinovsky, S. H. Batha and Z. Wang. Machine Learning for Detection of 3D Features using sparse X-ray Data. Submitted to *Review of Scientific Instruments*. (LA-UR-22-25023)

Reports

Nie, W. Solution-processed Perovskite Crystalline Films (SPeC). Unpublished report. (LA-UR-23-23032)

Presentation Slides

I. Falato, M. J., B. T. Wolfe, N. T. T. Nguyen-Fotiadis, X. Zhang and Z. Wang. Outer Shell Contour Extraction of ICF Images Using Deep Learning. Presented at *Conference on High Temperature Plasma Diagnostics (HTPD)*, Rochester, New York, United States, 2022-05-16 - 2022-05-16. (LA-UR-22-24438)

Nie, W. Low-dimensional Metal Halide Hybrid Perovskite Semiconductors for Light Emitting Devices. Presented at *Material Research Society, spring 2021*, Web meeting, New Mexico, United States, 2021-04-21 - 2021-04-27. (LA-UR-21-23773)

Nie, W. Emerging solution processible perovskite semiconductors for solid-state detectors. Presented at *3rd International Conferences on Nuclear Photonics, web meeting*, Online, Japan, 2021-06-07 - 2021-06-11. (LA-UR-21-25365)

Nie, W. Halide perovskite based opto-electronics: light emitting diodes and solid-state detectors. . (LA-UR-21-29270)

Nie, W. Carrier transport in 2D perovskite semiconductors and its application in high performance X-ray sensing. Presented at *Wake Forest University Department Colloqoium*, Winston-Salem, North Carolina, United States, 2022-10-06 - 2022-10-06. (LA-UR-22-30307)

Nie, W. Metal halide perovskites for photovoltaics and high performance radiation sensing. Presented at *Molecular* *foundry seminar*, Online, New Mexico, United States, 2022-10-04 - 2022-10-04. (LA-UR-22-30305)

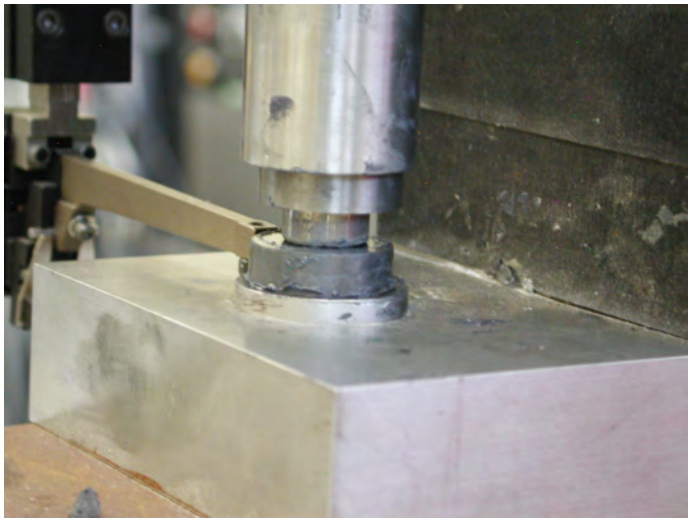
Wang, Z. Billion-pixel cameras for radiographic imaging & tomography. Presented at *Prompt Radiation detection and imaging workshop*, Las Vegas, Nevada, United States, 2022-04-25 - 2022-04-25. (LA-UR-22-23854)

Wang, Z. "6H" X-Ray Imaging Frontiers & Some Recent Highlights. . (LA-UR-22-26871)

**Peer-reviewed*

Modern Radiation Case Material for an Agile Complex

Kendall Hollis
20210536MFR



Alternative radiation case materials are being investigated under the LANL LDRD program to mitigate production cost and environmental impact while increasing manufacturing agility. Results from physics modeling has suggested several materials of interest. The image shows a test sample of a novel material being subject to a quasi-static compression test to determine material mechanical properties.

Project Description

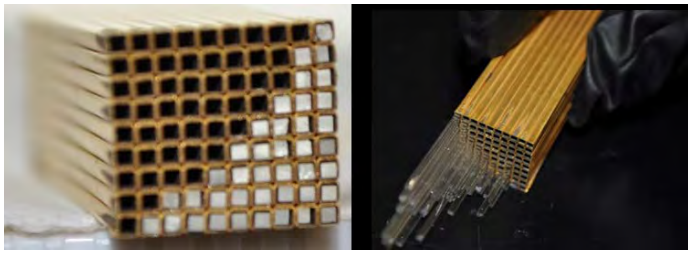
Evaluating new materials and technologies that were not available during cold war nuclear weapon development could provide future weapon systems with radiation cases that are lower in cost, lower in worker health risk and lower in environmental impact while delivering certified robust performance in a development and manufacturing time efficient manner. Using the latest available tools in physics modeling and material fabrication, this investigation will evaluate materials and recommend the most promising ones to be considered as alternatives to current materials and manufacturing technologies.

Technical Outcomes

This project was successful in demonstrating the feasibility of alternative materials for radiation cases. The goals of modeling performance of the materials and the entire system were met. Optimized compositions of materials were determined and these compositions were fabricated and tested. Manufacturing possibilities were investigated that could lead to substantial alleviation of current problems. In addition, as future conditions change, having alternative materials becomes even more important in the rapidly changing world.

High-Performance/-Precision/-Z (HPPZ) Scintillator Grids via Advanced Electrochemistry

Enkeleda Dervishi-Whetham
20210572MFR



Researchers at Sigma division fabricated a small-scale gold scintillator septa housing Lu2SiO5:Ce (LSO) crystals, to meet the detector performance requirements identified as targets by J-Division. High-Performance/-Precision/-Z(HPPZ) scintillator grids were found to exhibit a significant increase in detective quantum efficiency compared to steel grids, thereby providing higher image quality than present state of the art detectors. While chemical etching has produced good results in the past, the process is limited to a handful of materials. We expect that our proposed electrochemical method will allow us to fabricate grids from a diverse set of materials, while addressing mission needs at the Laboratory.

Project Description

Imaging is a critical element of measurements involving x-rays and other forms of non-visible probes to provide snapshots of dynamic events. Scintillators are used to convert the signal received to an electronic or visible signature. For spatial resolution, individual scintillators must be in a separated array, providing fine detail in closely spaced pixels with no cross-communication. Small (millimeter) scintillation crystals need to be spaced by micrometers, separated by very dense and high-atomic number materials. This is difficult or impossible to achieve through traditional techniques, and therefore is a major limitation of high-precision dynamic imaging. New pulse- and pulse-reverse electrochemical methods provide a pathway to solve this problem, and this project will demonstrate the application of these new methods to create high-precision micron-scale grids of gold and rhenium that can be scaled to any needed dimension. The development of practical methods to achieve high-precision large format future scintillators will have a major impact on advanced dynamic imaging needs. The end products will be useful to current mission needs and provide foundational research for other materials and applications. Further, the development of the technique itself will provide methods for processing dense, difficult to process materials, opening up other possible applications.

Technical Outcomes

The project demonstrated large-scale gold scintillator grid prototypes to meet the detector performance requirements identified as targets by the Dual-Axis Radiographic Hydrodynamic Test Facility. This technology was expanded to the development of other high-Z novel metal coatings such as Rhenium and Bismuth, as viable higher-performing, lower-cost solutions for imaging/detection and aerospace applications. Novel coatings will position the laboratory as a leader on development of high-Z materials and device fabrication, while addressing future engineering mission challenges.

Publications

Journal Articles

*Dervishi, E., M. McBride, R. Edwards, M. Gutierrez, N. Li, R. Buntyn and D. E. Hooks. Mechanical and tribological properties of anodic Al coatings as a function of anodizing conditions. 2022. *Surface and Coatings Technology*. **444**: 128652. (LA-UR-21-32123 DOI: 10.1016/j.surfcoat.2022.128652)

Hatfield, K. O., E. Dervishi-Whetham, D. R. Johnson, C. L. Clark, N. M. B. Brown and D. E. Hooks. Electrodeposition and Analysis of Thick Bismuth Films. Submitted to *Journal of Coatings Technology and Research*. (LA-UR-22-31417)

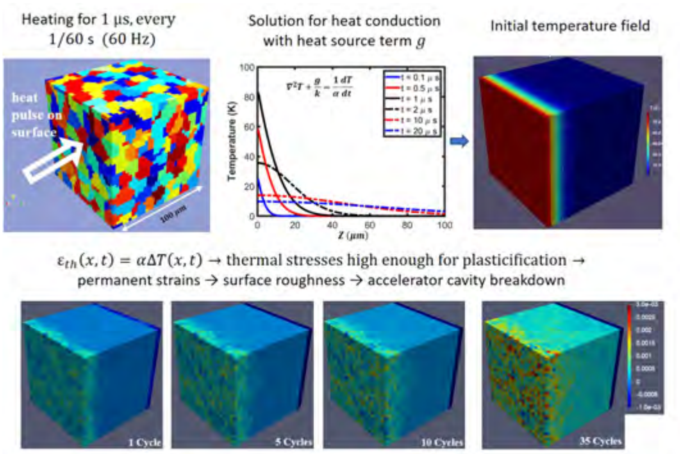
Presentation Slides

Dervishi-Whetham, E. High -Performance/-Precision/-Z(HPPZ) Scintillator Grids via Advanced Electrochemistry Phase I – Project # 20210572MFR- Mid year review. . (LA-UR-21-22404)

**Peer-reviewed*

Multiphysics Model for In-silico Design of Accelerator Materials with Higher Breakdown Thresholds

Ricardo Lebensohn
20220488MFR



Towards a multi-physics modelling framework for the in-silico design of new accelerator materials with higher breakdown and better resistance to thermal cycling. Top row shows temperature increase profiles computed from the solution of the heat conduction equation. Bottom row shows LANL's elasto-viscoplastic fast Fourier transform (EVPFFT) code predictions of strain normal to the surface after several heating and cooling cycles, in which a spatially and temporally varying thermal strain field is calculated using the coefficients of thermal expansion (CTE). Plastic strain accumulates with increasing number of cycles, causing out-of-plane displacements leading to surface roughness and breakdown.

Project Description

Accelerators are essential for executing key National Nuclear Security Administration missions. However, a technological barrier currently exists, preventing the delivery of new accelerators to meet future needs, due to limitations in the materials used to build accelerator cavities. In many mission problems, it is desirable to operate accelerators at high fields to enable high beam energies and/or short acceleration lengths. At high gradients, accelerator's structure materials operate under extreme conditions, including cyclic heating pulses and high electromagnetic fields. This leads to surface roughening and cracking due to thermal cycling caused by radio frequency (RF) losses, as well as to RF breakdown. Both can compromise the mechanical integrity of the cavities. In addition, RF breakdown disrupts the acceleration process. Understanding of the mechanisms responsible for breakdown, and developing new materials solutions (including composition/microstructure) is an important outstanding challenge that has resisted attempts so far. In this project, we will develop a novel microstructure-aware, multi-physics modelling framework to eventually enable the in-silico design of new accelerator materials with both higher breakdown thresholds and better resistance to thermal cycling.

Technical Outcomes

The project started the development of a novel and efficient multi-physics model based on Fast Fourier Transforms for polycrystalline materials subjected to cyclic heating and high electromagnetic fields. Once fully established, this computational tool will contribute to the mission problem as part of future in-silico design frameworks for new accelerator materials with higher breakdown thresholds.

Publications

Journal Articles

*Kube, C. M., Z. Feng, R. A. Lebensohn and M. Cherry. Resonant ultrasound spectroscopy for crystalline samples containing initial strain. 2022. *Journal of Applied Physics*. **131** (22): 225107. (LA-UR-22-25050 DOI: 10.1063/5.0091561)

Presentation Slides

Feng, Z., M. Zecevic, N. Rai, R. J. Mccabe, D. E. Hooks, M. Knezevic and R. A. Lebensohn. Surface roughness in polycrystalline copper under cyclic thermal loading: FFT-based thermomechanical modelling with experimental verification for accelerator applications. Presented at *TMS 2023 Annual Meeting & Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-24. (LA-UR-23-22600)

Feng, Z., M. Zecevic, R. J. Mccabe, D. E. Hooks, M. Knezevic and R. A. Lebensohn. Surface roughness in polycrystalline copper under cyclic thermal loading: FFT-based thermomechanical modelling with experimental verification for accelerator applications. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-19 - 2023-03-23. (LA-UR-22-26569)

Feng, Z., M. Zecevic and R. A. Lebensohn. Surface roughness in polycrystalline copper under cyclic thermal loading: FFT-based thermomechanical modelling with experimental verification for accelerator applications. . (LA-UR-22-27905)

Posters

Feng, Z., M. Zecevic, R. J. Mccabe, D. E. Hooks, M. Knezevic and R. A. Lebensohn. Surface Roughness in Polycrystalline Copper Under Cyclic Thermal Loading. . (LA-UR-22-27711)

**Peer-reviewed*

Design for Manufacture Pit Feasibility Study

Christina Scovel
20200665DI

Los Alamos will manufacture the components and parts for one pit that demonstrates Design for Manufacture (DfM) improvements. The project will also develop an integrated certification and qualification plan for this unit.

Project Description

This project will produce one or more prototype pits that demonstrate Design for Manufacture (DfM) improvements, as well as develop an integrated certification and qualification plan for the example DfM pit. The DfM approach could result in substantial savings of money, time, and waste in future pit production processes. If this project is a success it will impact the design of the new plutonium facility and the national strategy for pit development.

Technical Outcomes

This project accomplished its goal of demonstrating the integration of design with production. The project was also able to successfully produce one research prototype pit.

Publications

Presentation Slides

Gubernatis, D. C. Design for Manufacturing (DfM) Engineers Week Presentation. Presented at *LANL Engineers Week 2021*, Los Alamos, New Mexico, United States, 2021-02-23 - 2021-02-25. (LA-UR-21-21564)

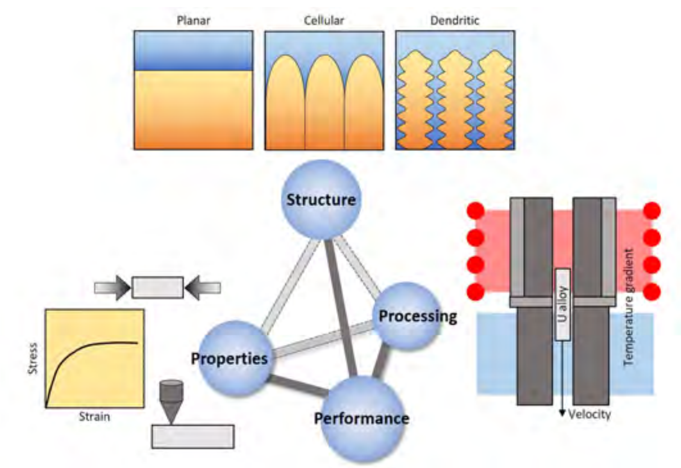
Mier, R. M. Rapid Prototyping of Forming Tools Through Additive Manufacturing. Presented at *DisrupTECH*, Los Alamos, New Mexico, United States, 2022-02-23 - 2022-02-23. (LA-UR-22-21011)

Rodriguez, D. J., A. S. Edgar, D. R. Vodnik and I. O. Usov. A Scalable Method for Rare Earth Oxide Thin Films by Chemical Solution Deposition. Presented at *American Vacuum Society (AVS) International Symposium and Exhibition*, Pittsburgh, Pennsylvania, United States, 2022-11-06 - 2022-11-11. (LA-UR-22-31297)

**Peer-reviewed*

Casting: Design Responsiveness and Rapid Qualification

Kara Luitjohan
20210692DI



The performance of manufactured parts relies on strong links between processing, structure, and properties. These relationships form a critical knowledge gap in uranium and uranium alloys, specifically post-solidification. Through a series of highly controlled experiments, these gaps will begin to be filled in for uranium-niobium alloys. A set of directional solidification and quenching experiments will be followed by microstructure characterization and mechanical testing to connect processing to structure to properties. Once established, these links will enable faster development periods for uranium parts, including higher flexibility in terms of processing and properties.

Project Description

The use of a cast part over a wrought (processed) part results in large savings in both time and money, therefore it is imperative to pursue approaches to control and optimize microstructural development during casting. This is critical for an agile, 21st century weapons complex. This project, by strengthening the processing-structure-property link in the area of solidification for uranium alloys, will allow new designs to be more responsive to mission needs. Furthermore, this will provide a significant step forward in being capable of designing for final properties while feeding back information on how to design components for ease of manufacturing. The broader mission of providing high quality uranium components for various research applications will also benefit from well-defined process-structure-property links.

Technical Outcomes

The project sought to generate and measure microstructures from highly controlled processing conditions and map these quantities to mechanical properties. The project successfully demonstrated the use of a new experimental setup for the production of highly controlled microstructures as well as developed and utilized a new framework for microstructural scale prediction for conditions outside of the bounds of the current project.

Publications

Journal Articles

Duan, T., Y. Shen, S. D. Imhoff, F. Yi, P. M. Voyles and J. H. Perepezko. Nucleation Kinetics Model for Primary Crystallization in Al-Y-Fe Metallic Glass. Submitted to *Journal of Chemical Physics*. (LA-UR-22-32384)

Presentation Slides

Imhoff, S. D. Direct Cast Modeling and Development. Presented at *Materials Compatability Review*, Los Alamos, New Mexico, United States, 2022-06-21 - 2022-06-21. (LA-UR-22-25533)

**Peer-reviewed*

Welding: Design Responsiveness and Rapid Qualification

Lindsay O'Brien
20210698DI

Design for a representative step jointed stainless steel hemisphere that will be hydroformed and machined for welding tests. Electron beam welding and gas metal arc welding will be used to test these parts to visualize and quantify the distortion post-welding. The results from these tests will be used an inputs into a weld model that will be able to predict how weld distortion develops from the heat input and residual stress inherent to welding. This is one of sixteen total designs for the project.

Project Description

The original welding and brazing methods and procedures used for pit production are being replaced rapidly due to new technology, aging of the materials used for decades, and more complete welding and joining science. New scientific approaches need to be developed in order to keep up with the programmatic demands for appropriately radiused test objects, future pit designs, and modifications to current designs. These same approaches are necessary in order to enhance legacy welds using new welding techniques and materials while still producing high quality, useful components. By utilizing the knowledge from past developments, including those from stockpile components, and combining it with modern techniques, such as blue light laser coordinate scanning, three-dimensional (3D) modeling, and finite element analysis, a method for accounting for weld distortion and its effect on overall component dimensions will be developed. A model for the deflection seen during welding will allow for more straightforward use of welding for test objects and more straightforward design changes in the future.

Technical Outcomes

The empirical model developed through the project represents the distortion observed in a part during welding, meeting the goal to implement modern tools such as finite element analysis into the welding process. This model, along with improved data collection capabilities, will help the team respond with agility to future Los Alamos missions. Going forward, these models will be applied to new welding processes and materials as well as to model distortion in other manufacturing techniques.

Publications

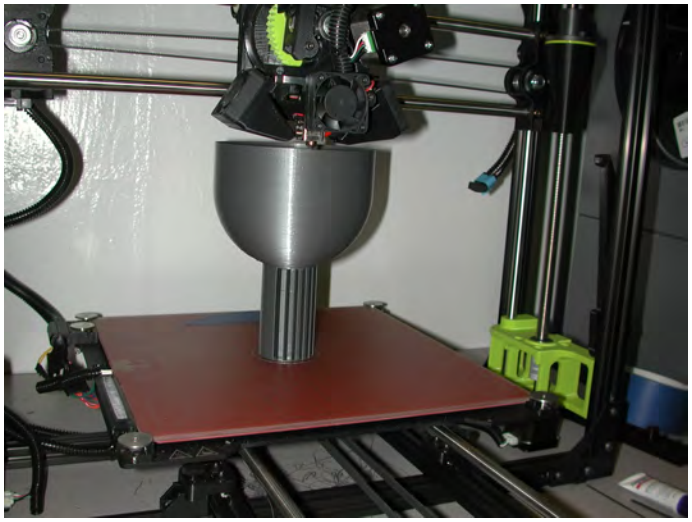
Presentation Slides

O'Brien, L. B. and A. N. Duffield. Development of a Weld Compensation Modeling Capability to Improve Design Agility. Presented at *JOWOG 28 Joining Subgroup Meeting*, Aldermaston, United Kingdom, 2022-08-22 - 2022-08-22. (LA-CP-22-20562)

**Peer-reviewed*

Powder Materials: Design Responsiveness and Rapid Qualification

Kendall Hollis
20210699DI



Example of a 3D printed mold master in the final stages of printing. Producing custom shaped mold masters which can be printed rapidly and dipped in a flexible material to form powder containing shapes allows for rapid production of powder pressed materials saving time, cost and valuable materials.

Project Description

This research advances the agile design, testing and manufacturing of Department of Energy (DOE) relevant materials and applications. Three-dimensional (3D) printing is used to bring modern advances to the production of powder processed materials. This will apply to all materials and parts produced by cold isostatic pressing.

Technical Outcomes

This project was successful in achieving the goals of demonstrating the feasibility of using additive manufacturing for fabricating tooling used in cold isostatic pressing of powders. Each of the specific goals of producing molds, mold masters and mold supports were met. This opens a new technique for quickly producing new part designs and also might be helpful to reduce manufacturing difficulties in future required part production.

Publications

Reports

Chen, C., J. C. Cooley, J. S. Carpenter and M. J. Kerr. Powder Materials: Design Responsiveness and Rapid Qualification. Unpublished report. (LA-UR-22-24781)

**Peer-reviewed*

The Effect of Defects on the Plutonium Gallium (PuGa) Phase Boundaries

Donald Brown
20210791DI

One of the goals of this project is to develop the protocol and relationships necessary to enable this and future research on plutonium (Pu) alloys. The Project Image shows a design schematic of the triple containment, one of four contained samples and a radiograph of a test container (containing iodine for contrast). The realization of the samples delivered in an approved containment is a significant accomplishment in that it demonstrates the establishment of the necessary relationships and presages a bright future of Pu measurements.

Project Description

As Plutonium Gallium (PuGa) components age in our enduring stockpile, spontaneous fission (alpha decay) events deposit defects in the microstructure. As in all metal alloys, these defects control the strength properties of PuGa and also effect the kinetics of phase transformations, potentially creating uncertainty in performance. This experimental work will collect data aimed at better understanding the effect of the defects on the phase transformations for the purpose of validating the development of microstructure aware models to be used in future performance calculations. Specifically, the delta-alpha transformation temperature will be determined with and without defects and the initiation sites for transformation will be directly observed. Also valuable equation of state data, i.e., the crystallographic thermal expansion, which is known to be hysteretic (depending on defects) will be determined over the measurement range.

Technical Outcomes

This project demonstrated the viability of high energy x-ray characterization of bulk plutonium gallium (PuGa) alloy samples at non-ambient conditions. The safety basis and trust to perform such measurements is now firmly established. Moreover, the ability to collect high quality statistical imaging and diffraction data which can be analyzed to determine quantitative microstructural features at bulk depths within the necessary three distinct layers of containment and additional two layers of sample environments has been established.

Publications

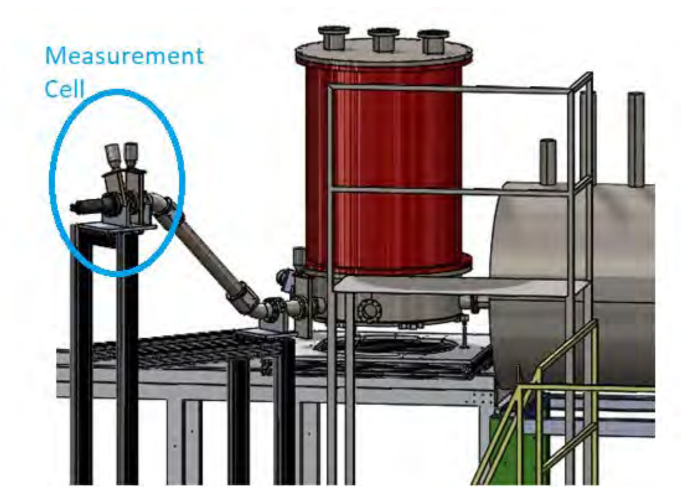
Presentation Slides

Carver, D. T., D. W. Brown, T. R. Jacobs, A. I. Smith, J. S. Park and P. Kenesei. High Energy X-Ray Characterization of Microstructure at Macroscopic Depths in Pu Alloys. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-20. (LA-UR-23-22757)

**Peer-reviewed*

New Technique for Uranium Hydride Analysis using Ultracold Neutrons

Zhaowen Tang
20210797DI



Schematic drawing of the measurement cell for surface hydrogen content measurements. The measurement cell will be connected to the ultracold neutron source. This project will look for the change in storage time of the cell before and after sample hydriding.

Project Description

Hydride formation in metals can lead to embrittlement of the material causing reduced ductility, decreased toughness, and fracture. Hydride formation in uranium (U) metal is particularly undesirable because it causes a 70% volume expansion of the metal lattice and the hydride corrosion product uranium hydride (UH3) is a friable, pyrophoric powder. We propose to use Ultracold Neutrons (UCNs) to probe surface hydrogen (H) distribution and accumulation, helping us to discern whether UH3 preferentially forms at the oxide/metal interface or in U metal, away from the interface. If these experiments are successful, the apparatus will also provide an important tool to study the effect of manufacturing process (e.g. various solidification technologies vs. wrought processing) on hydride corrosion susceptibility. A successful demonstration of this technique will be of interest to the National Nuclear Security Administration. The technique can also be expanded to other Uranium-based molecules, which will provide valuable data on surface hydride formation for nuclear fuel materials.

Technical Outcomes

The team performed a first hydrogen content measurement within the top 100 nanometer (nm) for depleted uranium (DU) samples using ultracold neutrons. The results show the concentration of hydrogen to be in excess of 0.18 mole/cubic centimeter in the first 89 nm of the sample. The team demonstrated that ultracold neutrons can very sensitively detect surface hydrogen content in real samples.

Publications

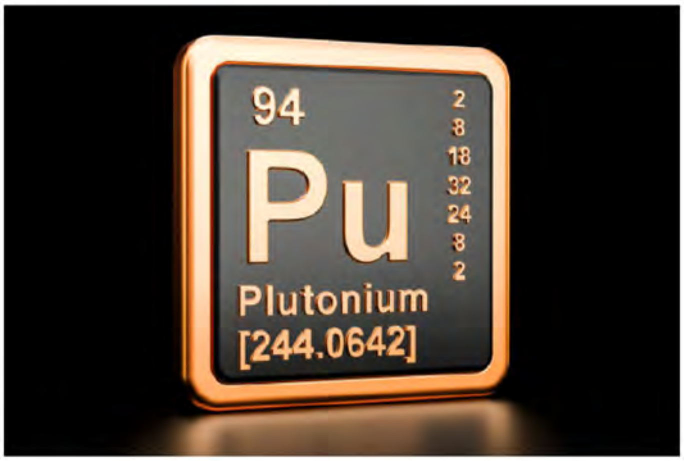
Presentation Slides

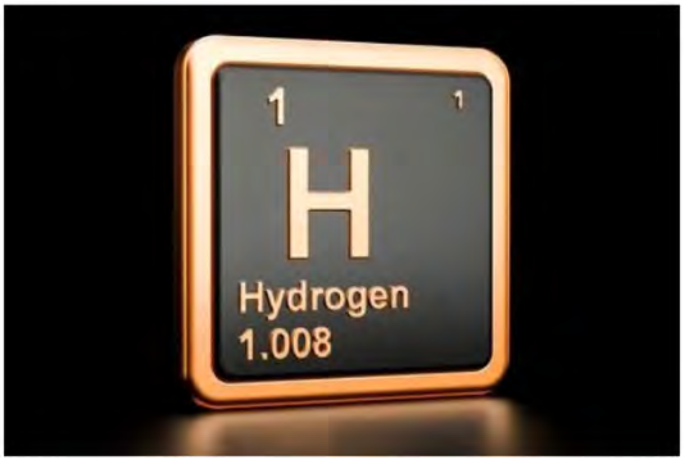
Ito, T. UCN Future at LANSCE. Presented at *LANSCE Future Spring Workshop*, Los Alamos, New Mexico, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-24476)

**Peer-reviewed*

An Investigation of Variables Affecting Plutonium Hydriding

Troy Holland
20210946DI





The project will model the intricacies of the plutonium/hydrogen system, including a handful of the many complications known to afflict the system such as alloy composition, impurities, processing, hydrogen isotope, and temperature.

Project Description

Our nuclear materials models are critical to enable efficient design decisions that maintain the safety, security, and reliability of the stockpile. Lack of adequate models moves some stockpile stewardship activities to the realm of impossible or prohibitively difficult/ expensive. Conversely, adequate computational models make necessary stockpile stewardship goals both possible and cost effective, while simultaneously keeping the nation's scientific capabilities as a whole at the global forefront.

Technical Outcomes

The project successfully furthered the state of the art in the areas of radiolytic gas chemistry, complex gas/surface chemical interactions, and radiolytic ion production/ transport effects.

Publications

Journal Articles

Gibson, T. R., V. M. Freixas, W. F. I. Malone, X. Li, H. Song, H. Negrin-Yuvero, A. J. White, D. V. Makhov, D. Shalashilin, Y. Zhang, N. Fedik, M. Kulichenko, R. A. Messerly, L. Mohanam, S. Fernandez-Alberti and S. Tretiak. NEXMD2 Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-23-20313)

*Messerly, R. A., B. J. Gifford and T. M. Holland. Kinetic isotope effects for dissociative recombination of tritiated ketenyl ion (3HCCO+): A surface-hopping ab initio molecular dynamics study. 2022. *Computational and Theoretical Chemistry*. **1210**: 113634. (LA-UR-21-29572 DOI: 10.1016/j.comptc.2022.113634)

Reports

Elliott, S. M. and T. M. Holland. Mechanisms and Isotope Effects in the Reverse Water Gas Shift. Unpublished report. (LA-UR-21-28598)

Newman, C. K. An Investigation of Variables Affecting Plutonium Hydriding (20210946DI): Surface Phase Transitions and Reactions. Unpublished report. (LA-UR-22-30182)

Posters

Fricke, C. H. and S. C. Hernandez. An irreversible poisoning - modeling the kinetics of water splitting on \xce\xb4-Pu surfaces using density functional theory. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21513)

**Peer-reviewed*

Bonded Interface Property Determination Using Nonlinear Ultrasonics

Timothy Ulrich
20220638DI

Project Description

Mechanical properties of bonded interfaces are critical to provide confidence in a system to perform as expected. Current methodologies can provide accurate and precise properties, however, have strong limitations on their applicability, especially when the materials may be difficult to handle or be embedded in a larger system. Advances in both measurement technologies and computational capabilities now allow for extending current techniques to reduce or remove the current limitations. The development of the proposed capability will greatly enhance nondestructive evaluation, manufacturing inspection and materials science with the ability to obtain the mechanical properties of systems and conditions in a manner not currently possible.

Technical Outcomes

The team learned that the stepped-sine input excitation used in typical laboratory experiments was computationally inefficient in simulations, precluding inversion for interface properties. Switching to white noise as a broadband excitation, the team resolved multiple simultaneously excited resonance modes within several hours of simulation. The simulated spectral peaks were verified against other numerical models. The team is now prepared to simulate nonlinear sample response under white-noise excitation for a suite of bonded interface parameters.

Publications

Reports

I. Ulrich, T. J., B. J. Euser and P. R. Geimer. Bonded Interface Property Determination Using Nonlinear Ultrasonics. Unpublished report. (LA-UR-22-29844)

Presentation Slides

Euser, B. J., P. R. Geimer and T. J. I. Ulrich. Bonded Interface Property Determination Using Nonlinear Ultrasonics. . (LA-UR-23-23099)

Geimer, P. R., L. B. Beardslee and T. J. I. Ulrich. Nonlinear resonant ultrasound spectroscopy with white-noise excitation. Presented at *International Symposium on Nonlinear Acoustics*, Oxford, United Kingdom, 2022-07-04 - 2022-07-08. (LA-UR-22-26125)

Geimer, P. R., L. B. Beardslee and T. J. I. Ulrich. Application of white-noise excitation for nonlinear resonant ultrasound spectroscopy. Presented at *Physical Acoustic Characterization for Material Assessment and Nondestructive evaluation*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-05. (LA-UR-22-27920)

I. Ulrich, T. J. Acoustic and Ultrasonic Resonance for Material Characterization and Nondestructive Evaluation Part I: Linear. . (LA-UR-22-26101)

**Peer-reviewed*

Seaborg Institute: Center for Advancing Actinide Science and Technology at Los Alamos National Laboratory

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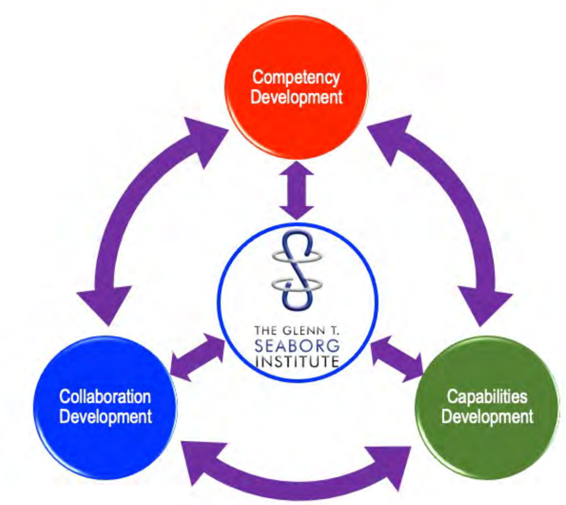

GTSI Leadership organizes strategic LDRD investments according to themes supporting the broad ranging actinide missions at Los Alamos National Laboratory. This model of coupled themes offers the greatest potential for cooperative function, innovation, and impact for LANL and the actinide research community, i.e., building a community and network beyond just actinide science. Competency Development is investment in workforce development to support and facilitate LANL building talent education and pipeline; Capability Development is investment in cutting edge science and technology via high-value high-risk high-payoff subprojects; and Collaboration Development is building an extensive internal and external network of direct research efforts.

Project Description

The Glenn T. Seaborg Institute project goal is intended to promote cutting edge ideas in actinide science, research and technology development with a focus on actinide competency and capability development with international collaboration relevant to all areas of Los Alamos National Laboratory (LANL) actinide mission space. This effort intersects with nuclear energy, nuclear weapons, and global security and will address the outstanding problems being identified and championed within the LANL Actinide Strategy Initiative via providing short-term seed money for postdocs, early career scientists and engineers to initiate research aimed at providing the competency and technical underpinnings necessary for multi-year projects; fostering sustained excellence and enhanced external visibility in relevant science; and establishing an intellectual community to facilitate the nucleation of ideas to solve timely and important relevant mission scientific and technological problems. Stakeholder federal agencies for Los Alamos actinide mission include Department of Energy (DOE)/ National Nuclear Security Administration (NNSA)/ Defense Programs, DOE/NNSA/Nuclear Nonproliferation, National Aeronautics and Space Administration (NASA), Department of Homeland Security (DHS)/Domestic Nuclear Detection Office (DNDO) and Department of Health and Human Services (DHHS). Mission Relevance includes Nuclear Security and National Defense, Energy Security, Environmental Management, and overall scientific discovery and innovation.

Publications

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Meeting and Exhibition, San Diego, California, United States, 2023-03-19 - 2023-03-23. (LA-UR-23-22554)

Posters

Carpenter, S. H., B. S. Billow, S. Sharma, A. Radovic, B. L. Scott, A. J. Gaunt, M. L. Neidig and A. Tondreau. Diastereoselective Template Synthesis on Iron and f-Block Elements. Presented at *Gordon Research Conference (GRC) - Inorganic Chemistry*, Newport, Rhode Island, United States, 2022-05-28 - 2022-06-03. (LA-UR-22-24944)

Ehrman, J. N., J. M. Kasper, X. Li, E. R. Batista and P. Yang. Quantum Mechanical Modeling of Actinyl Spectra. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-02. (LA-UR-22-27656)

Knapp, J. G., O. K. Farha, S. A. Kozimor, B. Stein and M. Y. Livshits. Photophysics and Resulting Photocatalysis of Uranyl-Organic Frameworks. Presented at *Gordon Research Conference (GRC) - Electron Donor Acceptor Interations*, Newport, Rhode Island, United States, 2022-07-31 - 2022-08-05. (LA-UR-22-27639)

Liao, C. H., J. M. Kasper, E. R. Batista, P. Yang and X. Li. Low-Scaling Perturbative Spin-Orbit Coupling in Closed-Shell TDDFT. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27669)

O'Brien, M. K., S. K. Lawrence, J. C. Cooley, B. Clausen and D. W. Brown. Investigating the Effect of Soluble Hydrogen on Plasticity in Uranium. Presented at *Plutonium Futures*, Avignon, France, 2022-09-26 - 2022-09-29. (LA-UR-22-29678)

Ordonez, O., A. J. Gaunt and T. W. Hayton. Neptunium-Ligand Multiple Bonding. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27452)

Patenaude, H. K., V. K. Mehta and F. J. Freibert. Oh, My Darling Clementine: A Contemporary Investigation of the Los Alamos Plutonium Fast Reactor. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-20985)

Robles, G., J. T. White, S. Widgeon Paisner and E. S. Sooby. Thermomechanical Performance of Al and Al2O3 Alloyed Fuel Composite U3Si2 + 50wt% UB2. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27678)

Roy, P. and A. Chen. Structural, optical and magnetic property of Uranium oxides. Presented at *Second International Workshop on Theory Frontiers in Actinide Science : Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-02-26. (LA-UR-23-22038)

Subedi, K. N. and R. M. Tutchton. Atomistic modeling of sodium borosilicate glasses containing uranium. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, SantaFe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21859)

Walusiak, B. W., A. I. Smith, S. S. Parker, S. C. Mann and C. L. Cahill. Characterization of Molten Salt Compounds Cs2UCl6 and Cs2UO2Cl4 From Room Temperature to Melting. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27856)

Walusiak, B. W., A. I. Smith, S. S. Parker, S. C. Mann and C. L. Cahill. Characterization of Molten Salt Compounds Cs2UCl6 and Cs2UO2Cl4 From Room Temperature to Melting. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-29776)

Walusiak, B. W., A. I. Smith, S. S. Parker, S. C. Mann and C. L. Cahill. Characterization of Molten Salt Compounds Cs2UCl6 and Cs2UO2Cl4 From Room Temperature to Melting. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-29823)

Other

Ehrman, J. N., J. M. Kasper, X. Li, E. R. Batista and P. Yang. Dataset of Exact Two-Component Multireference Configuration Interaction (X2C-MRCI) Calculations on Actinyls. Dataset. (LA-UR-22-29104)

Freibert, F. J. Glenn T. Seaborg, the US DOE Complex Actinide Mission, and the Seaborg Institute Network. Audio/Visual. (LA-UR-21-25387)

Schlimgen, A. W. Dataset of ab initio calculations on lanthanide and actinide molecules. Dataset. (LA-UR-21-21925)

**Peer-reviewed*

Rapidly Responding to Emerging Opportunities in Materials Science

Filip Ronning
20220533CR-IMS

The Institute for Materials Science Rapid Response Project aims to strengthen laboratory capability, develop new approaches that enable agile advances to national security challenges, and recruit, retain, and enhance critical skills for key, long-term mission objectives in broad support of the LANL Materials Strategy.

Project Description

The national security mission of Los Alamos National Lab will require new materials solutions to solve the problems that will arise in tomorrow's challenges. High risk/high reward ideas that can be quickly and efficiently explored are needed to identify opportunities for new growth areas. This project will pursue such projects within theoretical and experimental material science.

Publications

Journal Articles

Hunter Gordon, M. E., C. Huerta Alderete, F. A. Sauvage, A. Sone, A. T. Sornborger, P. J. Coles and M. V. S. Cerezo de la Roca. Inference-Based Quantum Sensing. Submitted to *Physical Review Letters*. (LA-UR-22-25337)

S. Cerezo de la Roca, M. V., L. Schatzki, M. Larocca and F. A. Sauvage. Theoretical Guarantees for Sn-Equivariant Quantum Neural Networks. Submitted to *Nature Communications*. (LA-UR-22-29899)

Conference Papers

Lin, Y. Quantum Neural Network Compression. Presented at *IEEE-International Conference on Computer-Aided Design*. (San Diego, California, United States, 2022-10-30 - 2022-10-30). (LA-UR-22-26425)

Reports

Chakraborty, S., D. J. Luscher and A. Hunter. A report on the development of a concurrent coupled Atomistic - Continuum model to predict the defect and grain structure for Additive Manufacturing process.. Unpublished report. (LA-UR-22-30131)

Erickson, K. and M. J. Monreal. IMS Rapid Response Project: The Synthesis of Discrete Uranium Nitrides on Inorganic Surfaces. Unpublished report. (LA-UR-22-29930)

Finkelstein, J. D. Rapid Response Summary Report. Unpublished report. (LA-UR-22-29903)

Lee, K. PHA-Based Next Generation Biodegradable Plastics. Unpublished report. (LA-UR-22-30118)

Martinez, U., L. A. Chavez Atayde, R. Castro and Y. Ge. Field-Enhanced Electrocatalysis of Durable Green Graphite Intercalated Compounds. Unpublished report. (LA-UR-22-30198)

Palmstrom, J. C. Elastoresistivity Measurements of Epitaxial Thin Film High Temperature Superconductors: IMS Rapid Response Roundup 2022. Unpublished report. (LA-UR-22-30207)

Ryu, C. Quantum Enhanced Atomic Gravity Sensor. Unpublished report. (LA-UR-22-30228)

Tutchton, R. M., C. A. Lane and J. Zhu. First-Principles Molecular Dynamics from Full-Potential Density Functional Theory. Unpublished report. (LA-UR-22-30188)

Wang, X. Probing interfacial and edge dynamics of van der Waals based heterostructures. Unpublished report. (LA-UR-22-30306)

Xu, H. Designing High-Entropy Single-Phase Zero-Thermal-Expansion Materials. Unpublished report. (LA-UR-22-30175)

Presentation Slides

El Atwani, O., M. R. Chancey and Y. Wang. Tri-Beam Irradiation Testing of Fusion Materials. . (LA-UR-22-30482)

Barros, K. M. Simulating Unconventional Magnetism. Presented at *36th Annual CSP Workshop*, Athens, Georgia, United States, 2023-02-20 - 2023-02-24. (LA-UR-23-21729)

Barros, K. M., A. Dahlbom, C. Miles, H. Zhang, S. Matin, M. S. Wilson, Y. W. Li, X. Bai, M. Mourigal and C. D. Batista. Sunny, an open source code for simulating generalized spin dynamics. Presented at *APS March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22457)

Chakraborty, S., D. J. Luscher and A. Hunter. Development of a concurrent coupled Atomistic - Continuum model to predict the defect and grain structure for Additive Manufacturing process. . (LA-UR-22-30084)

Erickson, K. and M. J. Monreal. IMS Rapid Response Project: The Synthesis of Discrete Uranium Nitrides on Inorganic Surfaces. . (LA-UR-22-29908)

Kim, J., N. S. Gupta and K. Lee. PHA-based Next Generation Biodegradable plastics. Presented at *IMS Rapid Response Roundup 2022*, Los Alamos, New Mexico, United States, 2022-10-05 - 2022-10-05. (LA-UR-22-30317)

Lin, Y. Intelligent Quantum Sensing with Quantum Neural Networks: an Application to Earthquake Detection. . (LA-UR-22-30266)

Martinez, U., L. A. Chavez Atayde, R. Castro and Y. Ge. Field-Enhanced Electrocatalysis of Durable Green Graphite Intercalated Compounds. Presented at *IMS Rapid Response Roundup 2022*, Los Alamos, New Mexico, United States, 2022-10-05 - 2022-10-05. (LA-UR-22-30210)

Palmstrom, J. C. Elastoresistivity Measurements of Epitaxial Thin Film High Temperature Superconductors. Presented at *IMS Rapid Response Roundup 2022*, Los Alamos, New Mexico, United States, 2022-10-05 - 2022-10-05. (LA-UR-22-30206)

Pettine, J. A., R. P. Prasankumar and H. Chen. Exceptional Points in Novel Multiscale Quantum-Nanoplasmonic Materials for Enhanced Sensing and Other Applications. . (LA-UR-22-30129)

S. Cerezo de la Roca, M. V. and C. Huerta Alderete. RR 2022-QS-1 Quantum Machine Learning for Quantum Sensing Slides. . (LA-UR-22-30163)

Ryu, C. Quantum enhanced atomic gravity sensor. . (LA-UR-22-30690)

Tutchton, R. M., C. A. Lane and J. Zhu. First-Principles Molecular Dynamics from Full-Potential Density Functional Theory. Presented at *IMS Rapid Responce Roundup*, Los Alamos, New Mexico, United States, 2022-10-05 - 2022-10-05. (LA-UR-22-30187)

Wang, X. Probing Interfacial and Edge Dynamics of Van der Waals Based Heterostructures. . (LA-UR-22-30304)

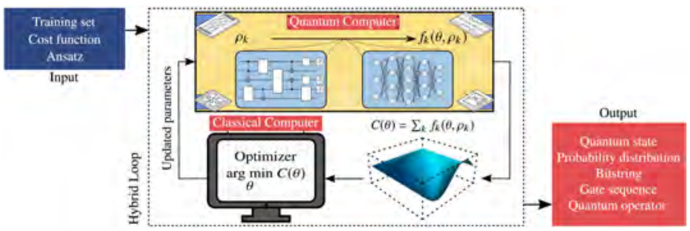
Posters

Ryu, C. and K. C. Henderson. Realization of a Gravity Gradiometer with a Waveguide Atom Interferometer. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-31 - 2022-06-03. (LA-UR-22-24819)

**Peer-reviewed*

Quantum Properties of Materials and Quantum Phenomena

Christopher Fryer
20220546CR-CNL



Schematic diagram of a variational quantum algorithm. The inputs to a variational quantum algorithm (VQA) are: a cost function C(theta), with theta a set of parameters that encodes the solution to the problem, an ansatz whose parameters are trained to minimize the cost and a set of training data {rho_k} used during the optimization. At each iteration of the loop, one uses a quantum computer to efficiently estimate the cost. This information is fed into a classical computer that leverages the power of optimizers to navigate the cost landscape C(theta) and solve the optimization problem.

Project Description

This project addresses fundamentals of quantum mechanics theory and the application of quantum computing methods to reveal the electronic properties of materials, including quantum materials, actinides, and photovoltaics, with emphasis on the development of new computational algorithms. We will explore quantum computing algorithms to study topological materials, superconductors, and to solve optimization problems using quantum computers. We will apply concepts and algorithms of quantum computation to understand the electronic structure of materials including complex correlated systems with entanglements, to explore novel functionality in topologically protected states, and to study materials relevant to high energy density applications under extreme conditions. This work has relevance in developing new materials for energy applications, modeling and predicting properties of f-electron matter, including actinides, for National Nuclear Security Administration mission objectives, and for developing new materials for quantum computing applications.

Publications

Journal Articles

*Cen, J., F. Correa, A. Fring and T. Taira. Stability in integrable nonlocal nonlinear equations. 2022. *Physics Letters A*. **435**: 128060. (LA-UR-21-32486 DOI: 10.1016/j.physleta.2022.128060)

Cen, J., R. Malla, W. J. de Melo Kort-Kamp and A. B. Saxena. Linearly driven non-Hermitian quantum systems. Submitted to *Physical Review A*. (LA-UR-22-31218)

Cen, J., Y. Joglekar and A. B. Saxena. PT and Anti-PT-symmetric Systems with Two Time-periodic Drives of Different Frequencies. Submitted to *Physical Review Research*. (LA-UR-22-31217)

Ecke, R. E. and O. Shishkina. Turbulent Rotating Rayleigh-B\xc3\xa9nard Convection. 2023. *Annual Review of Fluid Mechanics*. **55** (1): 603-638. (LA-UR-22-26951 DOI: 10.1146/annurev-fluid-120720-020446)

*Forde, A., V. M. Freixas, S. Fernandez-Alberti, A. J. Neukirch and S. Tretiak. Charge-Transfer Luminescence in a Molecular Donor-Acceptor Complex: Computational Insights. 2022. *The Journal of Physical Chemistry Letters*. **13** (37): 8755-8760. (LA-UR-22-28182 DOI: 10.1021/acs.jpclett.2c02479)

*Harris, J., B. Yan and N. A. Sinitsyn. Benchmarking Information Scrambling. 2022. *Physical Review Letters*. **129** (5): 050602. (LA-UR-21-30539 DOI: 10.1103/PhysRevLett.129.050602)

Kazi, S., M. V. S. Cerezo de la Roca and M. Larocca. Subspace controllability and failure of universality of Sn-equivariant k-body gates. Submitted to *NPJ Quantum Information*. (LA-UR-23-22003)

*Larocca, M., F. Sauvage, F. M. Sbahi, G. Verdon, P. J. Coles and M. Cerezo. Group-Invariant Quantum Machine Learning. 2022. *PRX Quantum*. **3** (3): 030341. (LA-UR-22-23371 DOI: 10.1103/PRXQuantum.3.030341)

Malla, R. K. Nonadiabatic dissociation of molecular condensates: competition between multi-mode reaction channels. Submitted to *Physical Review Letters*. (LA-UR-22-21329)

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*Malla, R. K. and M. E. Raikh. Landau-Zener transition between two levels coupled to continuum. 2022. *Physics Letters A*. **445**: 128249. (LA-UR-22-24335 DOI: 10.1016/j.physleta.2022.128249)

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S. Cerezo de la Roca, M. V., M. Ragone, P. Braccia, Q. T. Nguyen, L. Schatzki, P. J. Coles, F. A. Sauvage and M. Larocca. Representation Theory for Geometric Quantum Machine Learning. Submitted to *Quantum*. (LA-UR-22-30670)

S. Cerezo de la Roca, M. V., Q. T. Nguyen, L. Schatzki, P. Braccia, M. Ragone, P. J. Coles, F. A. Sauvage and M. Larocca. Theory for Equivariant Quantum Neural Networks. Submitted to *Physical Review X*. (LA-UR-22-30859)

Sharma, V., B. Bein, A. Lai, B. Pamuk, C. E. Dreyer, M. Fernandez-Serra and M. Dawber. Cooperative Interactions between Surface Terminations Explain Photocatalytic Water Splitting Activity on SrTiO3. 2022. *PRX Energy*. **1** (2): 023002. (LA-UR-22-20654 DOI: 10.1103/PRXEnergy.1.023002)

Sharma, V., L. A. Collins and A. J. White. Stochastic and Mixed Density Functional Theory within the projector augmented wave formalism for the simulation of warm dense matter. Submitted to *Physical Review Letters*. (LA-UR-23-20795)

Yan, B. and N. Sinitsyn. An adiabatic oracle for Grover's algorithm. Submitted to *Physical Review Letters*. (LA-UR-22-26707)

Conference Papers

Sauvage, F. A., Q. Nguyen, L. M. Schatzki, P. Braccia, M. J. Ragone, P. J. Coles, M. Larocca and M. V. S. Cerezo de la Roca. A Theory for Equivariant Quantum Neural Networks. Presented at *Quantum information Processing*. (Ghent, Belgium, 2023-02-04 - 2023-02-10). (LA-UR-22-29896)

Reports

Touil, A., F. Anza, S. Deffner and J. P. Crutchfield. Branching States as the Emergent Structure of a Quantum Universe. Unpublished report. (LA-UR-22-27917)

Presentation Slides

Cen, J., Y. Joglekar and A. B. Saxena. Double-driven Parity-Time (PT) and Anti-Parity-Time (APT) Symmetric Floquet Models. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21963)

Cen, J. and A. B. Saxena. Joint Parity-Time (PT) and Anti-Parity-Time (APT) Symmetric Qubits. Presented at *Quantum Fest 2021*, Mexico, Mexico, 2021-10-25 - 2021-10-29. (LA-UR-21-30560)

Forde, A. A. Solvation of Molecular Excited-States: (Non)-Equilibrium Transition Energies in Donor-Acceptor. Presented at *Sanibel Symposium*, St. Augustine, Florida, United States, 2023-02-12 - 2023-02-17. (LA-UR-23-21438)

Li, M., T. M. Sprouse and M. R. Mumpower. Nuclear Mass with Machine Learning and application to the astrophysical r-process. Presented at *Student Lightning Talk*, Los Alamos, New Mexico, United States, 2022-07-26 - 2022-07-27. (LA-UR-22-27174)

Malla, R. K. Coherent reaction between molecular and atomic Bose-Einstein condensates\xc2\xa0. Presented at *University of Massachusetts, Lowell*, Lowell, Massachusetts, United States, 2022-02-25 - 2022-02-25. (LA-UR-22-21677)

Malla, R. K. Ultrafast dynamics in Kane-Mele two-dimensional topological insulators. Presented at *APS March meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-14. (LA-UR-22-21966)

Sauvage, F. A., M. Larocca, Q. Nguyen, L. M. Schatzki, M. J. Ragone, F. M. Sbahi, G. Verdon, P. J. Coles and M. V. S. Cerezo de la Roca. Towards Geometric Quantum Machine Learning. . (LA-UR-22-32571)

Sharma, V., A. J. White and L. A. Collins. Mixing Stochastic-Deterministic Density Functional Theory in the PAW formalism to tackle extreme conditions physics. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22259)

Touil, A. Quantum Darwinism: the Origin of Objective Classical Reality. . (LA-UR-22-28130)

Posters

Forde, A. A., C. A. Mora Perez, S. Tretiak and A. J. Neukirch. Physical and Chemical Modifications of Nanomaterial-Chiral Molecule Interface for Enhanced Chirality-Transfer. Presented at *62nd Sanibel Symposium*, St. Augustine, Florida, United States, 2023-02-12 - 2023-02-17. (LA-UR-23-21201)

Li, M., T. M. Sprouse and M. R. Mumpower. Nuclear Mass with Machine Learning and application to the astrophysical r-process. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27126)

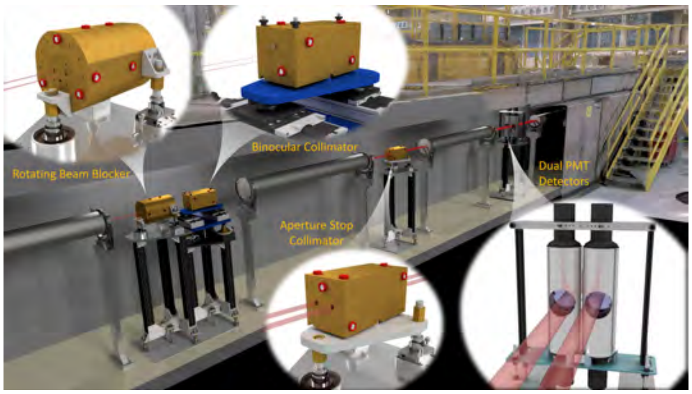
Malatesta, R. A., A. Piryatinski, E. Bittner and C. Silva Acu \xc3\xb1a. Probing quantum correlations in molecular systems with polarization-entangled photons. . (LA-UR-22-27659)

**Peer-reviewed*

Nuclear and Particle Futures

Predictive Understanding of Device Performance Through Innovative Measurement, Modeling, and Simulation on Radiochemical Dosimeters

Paul Koehler
20200108DR



The goal of the pictured Device for Indirect Capture Experiments on Radionuclides (DICER) is to make radiochemical diagnostics of nuclear devices more predictive by tightly constraining neutron-capture cross section for short-lived radionuclides. The unique, innovative dual-neutron-beam system created by the DICER collimation and detection apparatus minimizes both the sample size and experiment time, enabling measurements on samples 10,000 times smaller than typically used at other facilities. Radioisotopes for DICER are produced at the Isotope Production Facility at the Los Alamos Neutron Science Facility, and radiochemically separated and fabricated into samples at the Technical Area 48 hot cells.

Project Description

Radiochemical diagnostics (aka “radchem”) have been a crucial ingredient of nuclear weapons testing since inception, and efforts continue to this day to increase their usefulness and predictive capability. We will develop a novel, innovative technique to greatly reduce uncertainties for key radchem nuclear reaction rates, thereby enabling much more predictive understanding of nuclear weapons. Almost none of these rates have been measured and so they are very uncertain. Our main goal is to solve this problem by developing the first technique capable of determining key nuclear reaction rates with the required accuracy. Once demonstrated, this capability can be applied to many more cases of high interest to radchem as well as technical nuclear forensics and nuclear astrophysics, thus impacting additional Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions.

Publications

Journal Articles

Koehler, P. E., J. L. Ullmann, A. J. Couture and S. M. Mosby. Constraining the nuclear spin distribution using improved ^{197}Au neutron resonance parameters. 2022. *The European Physical Journal A*. **58** (10): 195. (LA-UR-22-28937 DOI: 10.1140/epja/s10050-022-00842-3)

Matyskin, A., A. Stamatopoulos, E. M. O'Brien, B. J. DiGiovine, V. Mocko, M. E. Fassbender, C. Vermeulen and P. E. Koehler. Production of zirconium-88 via proton irradiation of metallic yttrium and preparation of target for neutron transmission measurements at DICER. Submitted to *Scientific Reports*. (LA-UR-22-28588)

Stamatopoulos, A., A. J. Couture, B. J. DiGiovine, P. E. Koehler and G. Y. Rusev. A Large Area Picosecond Photodetector for neutron transmission measurements at DICER at LANSCE. Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-22-31612)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, A. Matyskin, V. Mocko, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. DICER: A new instrument for nuclear data for nuclear security. Submitted to *Journal of Radioanalytical and Nuclear Chemistry*. (LA-UR-22-22946)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. New capability for neutron transmission measurements at LANSCE: The DICER instrument. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-21-29960)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. New apparatus for neutron capture measurements on extra small radioactive samples: The DICER instrument at LANSCE. Submitted to *Neutron News*. (LA-UR-22-21702)

Stamatopoulos, A., P. E. Koehler, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, V. Mocko, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. The new Device for Indirect Capture Experiments on Radionuclides at LANSCE: Efforts on measuring the resonance(s) responsible for the extremely large 88Zr(n,g) cross section. Submitted to *EPJ Web of Conferences*. (LA-UR-22-29884)

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Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. A new approach for indirect capture measurements:The DICER neutron transmission station at LANSCE. Presented at *Hellenic Nuclear Physic Society Symposium 2021 (HNPS2021)*. (Athens, Greece, 2021-09-24 - 2021-09-25). (LA-UR-21-32022)

Reports

Schatz, H., A. D. Becerril Reyes, A. Best, E. F. Brown, K. Chatziioannou, K. A. Chipps, C. M. Deibel, R. Ezzeddine, D. K. Galloway, C. J. Hansen, F. Herwig, A. P. Ji, M. Lugaro, Z. Meisel, D. Norman, J. S. Read, L. F. Roberts, A. Spyrou, I. Tews, F. X. Timmes, C. Travaglio, N. Vassh, A. J. Couture, C. L. Fryer, A. E. Lovell, M. R. Mumpower and T. M. Sprouse. Horizons: Nuclear Astrophysics in the 2020s and Beyond. Unpublished report. (LA-UR-22-29206)

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Couture, A. J. LANSCE: World's Brightest Time-of-Flight Neutron Source for Nuclear Physics. Presented at *NSAC Long Range Plan Town Hall Meeting on Nuclear Structure Reactions and Astrophysics*, Lemont, Illinois, United States, 2022-11-14 - 2022-11-14. (LA-UR-22-32062)

Couture, A. J., P. E. Koehler, H. Y. Lee, S. A. Kuvin, B. J. DiGiovine, P. Gastis, A. Georgiadou, D. G. J. Votaw, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, V. Mocko, G. Perdikakis and P. Tsintari. Directly measured neutron-induced reactions on radioactive nuclides for Nuclear Astrophysics. Presented at *American Physical Society (APS) April Meeting*, New York, New York, United States, 2022-04-09 - 2022-04-13. (LA-UR-22-23195)

DiGiovine, B. J. Enabling direct reaction studies with small, highly radioactive samples. Presented at *Workshop for Applied Nuclear Data Activities 2022*, Cisco WebEx (Virtually), New Mexico, United States, 2022-02-28 - 2022-02-04. (LA-UR-22-21560)

Erjavec, T., J. L. Ullmann and P. E. Koehler. ARTIE: Measuring the 57keV neutron cross-section of liquid argon. Presented at *APS Far West Section (remote)*, Davis, California, United States, 2020-10-10 - 2020-10-10. (LA-UR-20-30192)

Koehler, P. E. DICER (Device for Indirect Capture Experiments on Radionuclides). Presented at *Nuclear Data Advisory Group*, santa fe, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21109)

Koehler, P. E. New Opportunities with Neutron Transmission and Capture. Presented at *Paul Koehler*, none (Webex), New Mexico, United States, 2022-10-17 - 2022-10-18. (LA-UR-22-30806)

Koehler, P. E., T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, J. M. O'Donnell, R. Reifarth, G. Y. Rusev, A. Stamatopoulos and J. L. Ullmann. 149Sm Results from DICER Plus DANCE. Presented at *Nuclear Data Advisory Group*, new york,

New York, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31180)

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Pagani, L., S. Andringa, Y. Bezawada, T. Erjavec, J. He, J. Huang, P. E. Koehler, M. J. Mocko, M. Mulhearn, E. Pantic, L. Pickard, R. Svoboda, J. L. Ullmann and J. Wang. ARTIE (near)-final results. Presented at *DUNE collaboration meeting (remote)*, none, California, United States, 2020-09-23 - 2020-09-23. (LA-UR-20-29932)

Rusev, G. Y., E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, C. E. Fry, M. Jandel, P. E. Koehler, S. M. Mosby, C. J. Prokop, A. Stamatopoulos and J. L. Ullmann. Neutron Resonance Parameters of 191Ir and 193Ir. Presented at *2022 Fall Meeting of the Division of Nuclear Physics of the American Physical Society*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-30. (LA-UR-22-31239)

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Stamatopoulos, A. DICER: A new instrument at LANSCE to study tiny radioactive samples. . (LA-UR-22-31351)

Stamatopoulos, A. DICER: a new device to constrain (n,\xce\xb3) rates on tiny radioactive samples through innovative transmission experiments. Presented at *NSAC long range plan town hall*, Lemont, Illinois, United States, 2022-11-14 - 2022-11-16. (LA-UR-22-31895)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, A. Matyskin, V. Mocko, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. The new Device for Indirect Capture Experiments on Radionuclides at LANSCE: Efforts on measuring the resonance(s) responsible for the extremely large 88Zr(n,\xce\xb3) cross section. Presented at *International Conference on Nuclear Data for Science and Technology*, Sacramento, California, United States, 2022-07-24 - 2022-07-29. (LA-UR-22-27115)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, A. Matyskin, V. Mocko, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. Experimental setup and preparation for the indirect measurement of 88Zr(n,\xce\xb3) at DICER at LANSCE\xc2\xa0. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Nuclear Physics (DNP)*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-30. (LA-UR-22-30807)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, E. M. Bond, T. A. Bredeweg, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, V. Mocko, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. DICER: A new instrument for nuclear data for nuclear security. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kona, Hawaii, United States, 2022-04-03 - 2022-04-08. (LA-UR-22-23185)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. A new approach for indirect capture measurements: The DICER neutron transmission station at LANSCE. Presented at *HNPS2021*, Athens, Greece, 2021-09-24 - 2021-09-25. (LA-UR-21-29104)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. A Large Area Picosecond Photo Detector for neutron transmission measurements at DICER at LANSCE. Presented at *16th International Conference on Scintillating Materials & their Applications*, Santa Fe, New Mexico, United States, 2022-09-19 - 2022-09-23. (LA-UR-22-29702)

Stamatopoulos, A., P. E. Koehler, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. New capability for indirect neutron capture measurements: The DICER instrument at LANSCE. Presented at *Nuclei in the Cosmos 2021*, Chengdu, China, 2021-09-21 - 2021-09-25. (LA-UR-21-29183)

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Stamatopoulos, A., P. E. Koehler, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, S. D. Essenmacher, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, V. Mocko, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. DICER: Device for Indirect Capture Experiments on Radionuclides. Presented at *LANSCE User meeting 2022*, Los Alamos, New Mexico, United States, 2022-06-02 - 2022-06-03. (LA-UR-22-24925)

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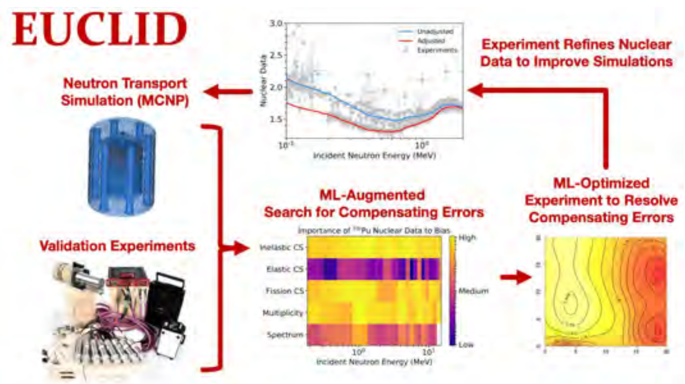
**Peer-reviewed*

Revolutionary Advances in Nuclear Data to Underpin LANL 21st Century Missions

Jesson Hutchinson
20210021DR



Compensating errors within nuclear data can adversely impact application simulations, but cannot be resolved using current techniques. EUCLID aims to provide a capability to reduce these compensating errors. In order to achieve this, we utilize machine learning (ML) with simulated sensitivities in Monte-Carlo N-particle (MCNP) of experiments and measured results to augment expert identification of areas where compensating errors may be resolved. The design of new experiments will then be optimized using ML to target these compensating errors. After the new experiments are completed, the new data are used to produce adjusted libraries with reduced compensating errors while accounting for physics constraints.

Project Description

Nuclear data and simulation advancements are important to the Los Alamos National Laboratory (LANL) mission. The work in the EUCLID (Experiments Underpinned by Computational Learning for Improvements in nuclear Data) project is an important step towards long-term mission needs. One major goal of EUCLID is to reduce compensating errors in nuclear data that impede our predictive capabilities. This first-of-a-kind capability builds upon renowned LANL strengths in nuclear-data evaluation, transport codes, validation experiments, and machine learning. If successful, the advancements of this work will have cross-cutting impact which can be applied to answer urgent mission needs representing national security challenges for the Laboratory's Plutonium Facility (PF-4) pit production, Design for Manufacturing, Enhanced Capabilities for Subcritical Experiments (ECSE), Weapons and global security assessments, and micro-reactor design.

Publications

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Cutler, T. E., K. M. Amundson, J. D. Hutchinson and N. W. Thompson. Analysis of Major Benchmark Uncertainties for Fast Metal Assemblies in the ICSBEP Handbook. Submitted to *Nuclear Science and Engineering*. (LA-UR-22-27049)

Grosskopf, M. J., S. A. Vander Wiel and D. Neudecker. On Pathologies in Estimating the Mean with Relative Systematic Uncertainties. Submitted to *American Statistician*. (LA-UR-22-32397)

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Kodeli, I., M. Fleming, O. Cabellos, L. Leal, Y. Celik, Y. Ding, B. Jansky, D. Neudecker, E. Novak, S. Simakov, Y. Iwamoto and A. Valentine. Outcomes of WPEC SG47 on "Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation". Submitted to *EPJ Web of Conferences*. (LA-UR-22-27759)

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Posters

Bell, B. W., T. Mark, D. Neudecker, M. J. Grosskopf and J. D. Hutchinson. Applying PCA to Random Forest Analysis to Tease Out Correlated Data When Predicting Bias in Integral Experiments. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-22095)

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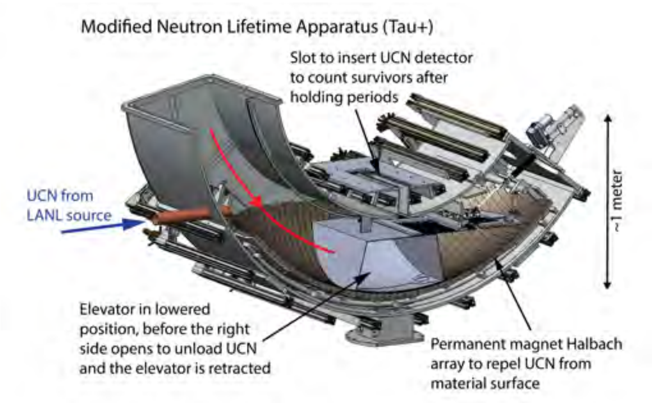
**Peer-reviewed*

Beyond the Standard Model through Precision Neutron Decay

Steven Clayton
20210041DR



Precision measurements of beta decay observables test the standard model of particle physics, with neutron beta decay a particularly clean example as nuclear structure corrections are not needed. The Tau+ experiment will extend the world-leading ultra-cold neutron (UCN)tau experiment another factor of three in precision reach by increasing the number of observed neutrons an order of magnitude through a novel "elevator" loading method, shown in the figure.

Project Description

The standard model of particle physics is an extremely successful theory that describes the interactions of subatomic particles, however the theory appears to be incomplete as it does not predict some of the fundamental observed properties of the universe, such as the predominance of matter over antimatter. Modifications to the standard model theory can explain these observations, while also implying the existence of new subatomic particles. This project aims to test the standard model at very high precision through measurement of the radioactive decay of the neutron, which could reveal the presence of additional subatomic particles or otherwise provide stringent constraints on new theories. The neutron is a constituent of the atomic nuclei of everyday matter. When free from an atomic nucleus, the neutron is unstable and decays after an average of 15 minutes into a proton, electron and antineutrino. This project will develop experiments to improve measurements of two properties of neutron decay, perform state-of-the-art theoretical calculations to interpret results in terms of the standard model, and evaluate constraints on beyond standard model theories.

This effort is well-aligned with the Department of Energy (DOE)-Office of Science goal of determining the new standard model of particle physics.

Publications

Journal Articles

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Yoo, J., R. Gupta, T. Bhattacharya, B. Yoon, S. Mondal and E. Mereghetti. Electroweak box diagrams on the lattice for pion and neutron decay. Presented at *The 39th International Symposium on Lattice Field Theory*, Bonn, Germany, 2022-08-08 - 2022-08-13. (LA-UR-22-28091)

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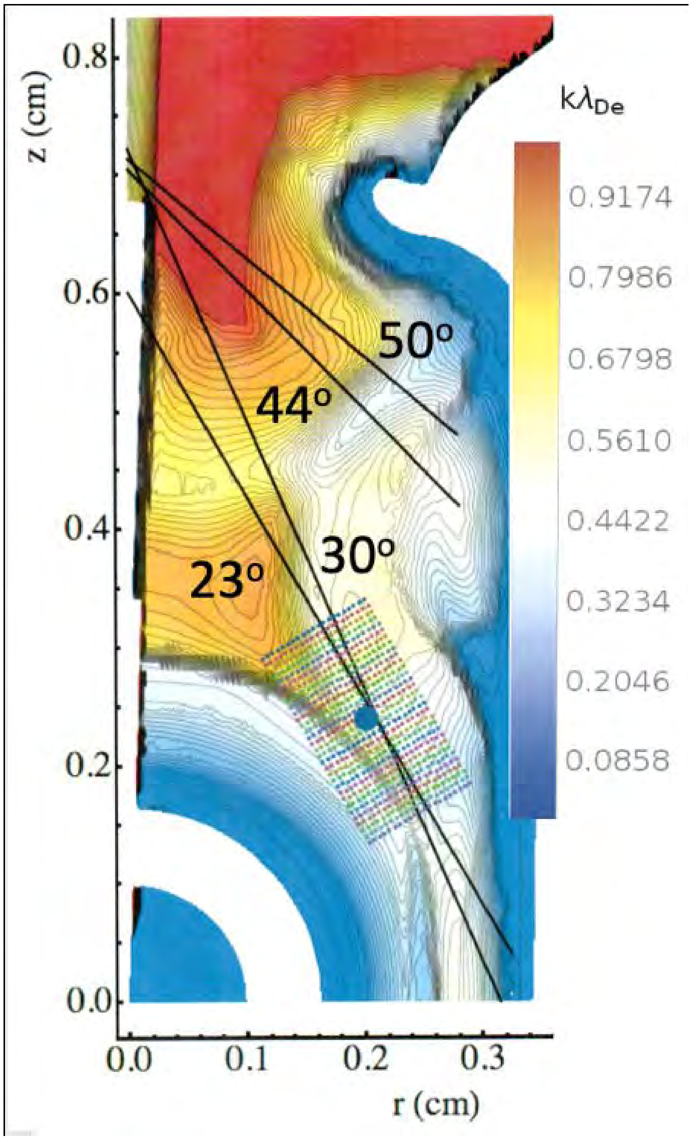
**Peer-reviewed*

High-fidelity Electromagnetic Simulation Capability for Inertial Confinement Fusion (ICF)/High Energy Density (HED) Experiments

Luis Chacon
20210063DR



The hohlraum is a metallic cylinder that surrounds the capsule in Inertial Confinement Fusion. It transforms laser energy into X-rays, which then drive the capsule by ablation. Hohlraums plasma environments are not amenable to a radiation-hydrodynamic description, and require higher fidelity models (the goal of this LDRD project). The figure shows the hohlraum plasma after laser irradiation. The plasma is color-coded such that red regions are hot and rarefied, and blue regions are cold and dense. Laser-beam propagation angles are indicated, as is the area suffering from laser-plasma interactions, of particular interest for this project.

Project Description

This project intends to develop and demonstrate a high-fidelity simulation capability for High Energy Density (HED) and Inertial Confinement Fusion (ICF) experiments. The proposed work is critically important for the United States national security and the Los Alamos National Laboratory mission. Achieving ICF ignition in the laboratory remains critical for the stockpile stewardship program. This project will have a direct mission impact not only by assessing paths towards ignition, but also by enabling new understanding of HED experiments that use hohlraums and similar environments.

Publications

Journal Articles

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Chacon, L. Modern implicit algorithms for multiscale kinetic plasma simulation. Presented at *2nd Computational Physics School for Fusion Research*, Virtual, Massachusetts, United States, 2021-08-30 - 2021-08-30. (LA-UR-21-28346)

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Posters

Chen, G., L. Chacon, A. J. Stanier, B. Philip and S. E. Anderson. A multiscale hybrid Monte-Carlo-Gaussian Coulomb-Collision Algorithm for Hybrid Kinetic-Fluid Simulations. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30577)

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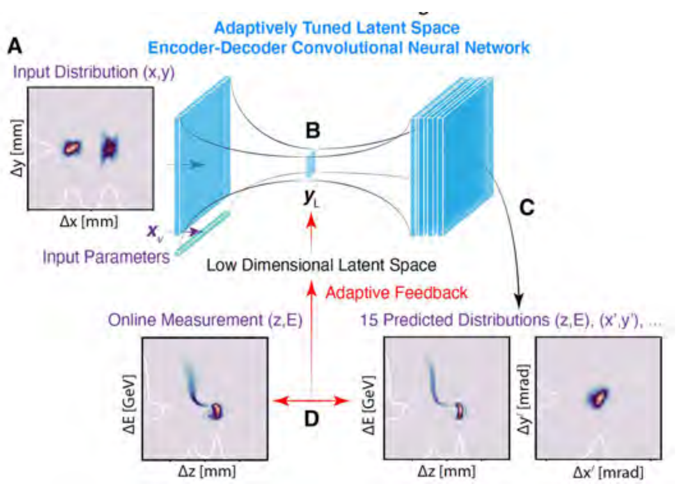
**Peer-reviewed*

Charged Particle Beam Control and Diagnostics using Adaptive Machine Learning

Alexander Scheinker
20220074DR



An example of adaptive machine learning for time-varying particle accelerator dynamics is shown using convolutional neural networks to map input beam distributions and vectors of accelerator parameters (>10k dimensional input), down to a two-dimensional (2D) latent space (B) before reconstructing the 2D projections of a beam's 6D phase space (C) while satisfying physics constraints and correlations between dimensions. The (z,E) projection is then compared to online measurements guiding model independent adaptive feedback (D) acting on the latent space representation to track all of the 6D phase space projections while the accelerator's unknown input beam distribution and components vary with time.

Project Description

The Department of Energy (DOE) utilizes some of the world's most advanced particle accelerators for research and development. The Los Alamos Neutron Science Center (LANSCE) provides intense proton and neutron beams for basic material science, weapons, and basic science research, the dual axis radiographic hydrodynamic test facility (DARHT) provides X-rays for imaging of explosive dynamics, and the Linac Coherent Light Source (LCLS) provides extremely bright and short X-ray pulses for studying everything from biological processes to shock waves in materials relevant to DOE programs. These facilities face major challenges in tuning and operations. LANSCE and DARHT require weeks to start up after maintenance and to switch between experiments. In 2015 the LCLS spent >400 hours on tuning the machine, which is equivalent to 10 experiments and costs $12M in operational budget. The goals of this work are to improve such facilities by providing fast, automated and optimal tune up and operation, providing higher scientific throughput and higher quality beams to all users. We will also develop new capabilities, such as non-invasive diagnostics and adaptive machine learning-based algorithms to provide higher quality beams than is currently possible to enable future Department of Energy capabilities such as Los Alamos National Laboratory's planned Dynamic Mesoscale Material Science Capability.

Publications

Journal Articles

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Scheinker, A., F. Cropp and D. Filippetto. Adaptive latent space tuning for robust ML beyond the training set with application to 6D phase space diagnostics for a time-varying UED compact accelerator. Submitted to *Physical Review E*. (LA-UR-23-20233)

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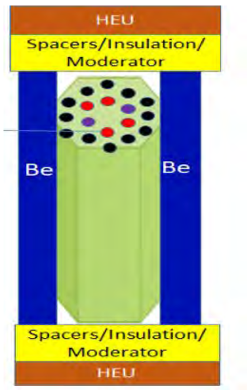
**Peer-reviewed*

Next Generation Small Nuclear Reactors

Holly Trellue
20220084DR



By establishing a combination of matrix moderator materials and low enriched uranium in a traditional criticality experiment geometry with high enriched uranium, expansion of current capabilities to low-enriched uranium currently required for small reactor designs can be performed.

Project Description

Traditional space reactor designs use high enriched uranium as fuel to attain the most efficient power production possible at small core sizes. As small/space reactors transition away from high enriched uranium to high assay low-enriched uranium, infrastructure and materials required for low enriched-fueled systems need to be developed such that power can still be obtained from a reasonably-size system. For instance, to help slow neutrons down and increase fissionability/energy production from as small a core as possible, moderating material is required. This project will explore an innovative moderator matrix material with coated particulate fuel to achieve optimal safety, criticality, and materials features for small reactor designs. It will also estalish criticality testing methodologies useful for reducing risk while building reactors for low-enriched uranium (LEU) high assay (HALEU) fuel and increase simulation efficiency in modeling particulate fuel with a premier Monte Carlo neutron transport code widely used for small reactor design calculations. Such capability development will then be transitioned to projects with reactor vendors and/or Deparment of Energy- Nuclear Energy and Department of Defense programs to advance reactor design and testing applications appropriately nationwide.

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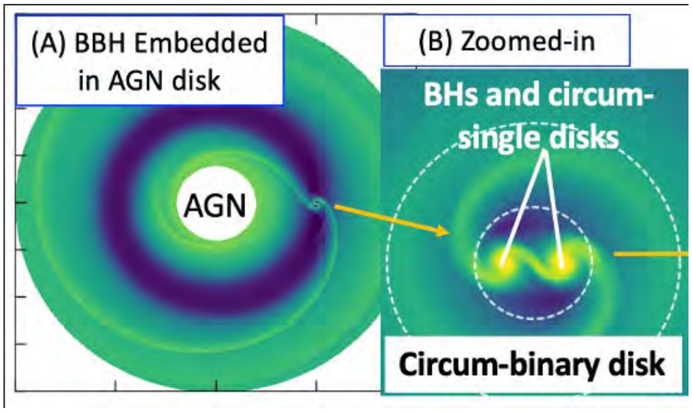
**Peer-reviewed*

Solving the Mystery of Laser Interferometer Gravitational-Wave Observatory (LIGO) Heavyweight Mergers: New Windows on Gravitational Wave Science in the Multi-Messenger Era

Hui Li
20220087DR



When a binary black hole (BBH) is embedded inside a disk around an active galactic nuclei, it will regulate the material around its orbit in such a way that a hierarchical structure of various disks will emerge, including the circum-single and circum-binary disks. This work will study whether these BBHs will produce gravitational waves and whether there will be optical counterparts that can be observed. The LIGO observations are providing unique constraints to test our theoretical modeling.

Project Description

The gravitational wave (GW) observations have discovered new sources that defy traditional explanation, even inconsistent with conventional models. We propose a new theory that some GW sources come from binary black holes in disks around supermassive black holes. Using the state-of-the-art tools developed at Los Alamos National Laboratory, we will carry out comprehensive studies on this new theory to examine the detailed physical processes and predict what the expected observations would be. We will also perform rapid follow-up observations of GW sources to test our theory. These studies will develop and utilize tools that will benefit National Nuclear Security Administration (NNSA) missions, as well as help developing early career scientists who will contribute to NNSA missions.

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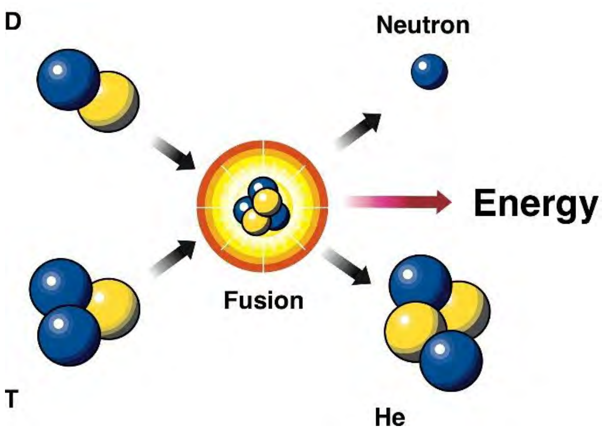
**Peer-reviewed*

First Steps Towards a New Experimental Platform to Study Burning Plasmas

William Daughton
20220113DR



In hot thermonuclear plasmas, isotopes of hydrogen (D = deuterium and T = tritium) can undergo fusion reactions resulting in the production of neutrons and helium (He) and the release of energy. This project will investigate an experimental concept to achieve the required plasma conditions. Image is from - https://www.energy.gov/science/doe-explainsnuclear-fusion-reactions

Project Description

The development of an experimental platform to study the physics of robustly burning plasmas has been a longstanding goal of the Department of Energy/National Nuclear Security Administration. Such experiments would enable researchers to probe the nonlinear physics of thermonuclear burn and to further validate our simulation tools for stockpile stewardship activities. This project will perform experiments to better understand the feasibility of a concept for producing the necessary conditions. These new measurements will allow researchers to validate computer simulations and further refine the concept. These efforts will demonstrate a path forward for future fusion experiments.

Dark Matter Detection with Quantum Materials

Daniele Spier Moreira Alves
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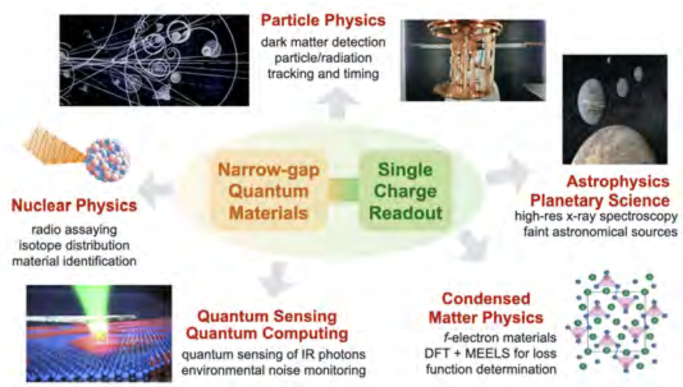

The development of quantum sensing detectors using LANL's novel narrow gap semiconductors will enable the exploration of currently inaccessible parameter space of dark matter models. In the long term, this novel detector technology could also find applications in numerous fields of science and industry, as outlined in the Figure.

Project Description

About 85% of the total mass in the Universe consists of dark matter, yet little is known about its particle properties such as mass and interactions with ordinary matter. The only way to answer some of the most basic questions about the nature of dark matter is to detect it in laboratory experiments. Unfortunately, many theories predict that dark matter particles are able to deposit only tiny amounts of energy in a detector, and are outside the sensitivity of existing detector technology. The goal of this project is to develop ultra-sensitive detector technology to probe currently inaccessible theories of dark matter. The enabling innovation are novel semiconducting materials with quantum sensing applications discovered Los Alamos National Laboratory. We will demonstrate the unprecedented sensitivity of these detectors to quantum sensing regimes in the infrared range, and with an order of magnitude improvement in energy resolution over current semiconductor-based detector technology. The development of these new particle and radiation detectors can have a significant impact in numerous areas of science and industry, including dark matter detection, astrophysics and planetary science, and quantum sensing. All of these areas are aligned with national priorities of the Department of Energy Office of Science, National Aeronautics and Space Act, and the National Quantum Initiative.

Publications

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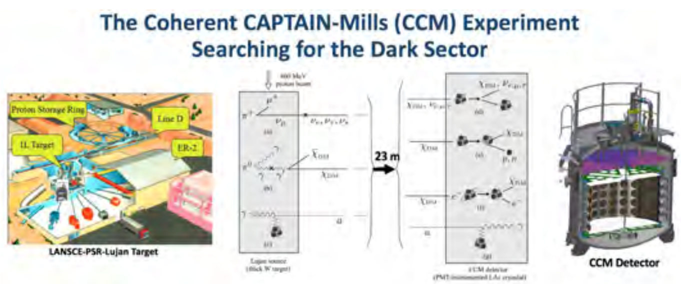
**Peer-reviewed*

Searching for Coherent Neutrinos and Dark Matter with the Coherent Captain-Mills Experiment

Richard Van De Water
20220795DR



The Coherent CAPTAIN-Mills (CCM) experiment will search for dark sector particles at the LANSCE Lujan center. The LANSCE accelerator directs an intense proton beam on a tungsten target that generates possible dark sector particles that can be detected by the sensitive liquid argon CCM detector. This will probe for new physics such as sterile neutrinos, dark matter, and axion particles that can account for the missing matter in the Universe. Such a discovery would be revolutionary and stimulate new theories on the origins and evolution of the Universe.

Project Description

The Coherent CAPTAIN-Mills (CCM) is a new experiment designed to search for coherent neutrinos and dark sector physics such as dark matter and axions. This project will commission the filtration and recirculation system, which is crucial to increasing the detected scintillation light efficiency, thereby decreasing the detection threshold to the level of approximately 10 Kiloelectron-volts (keV). This is necessary for efficient low energy event detection to detect neutrino and dark matter coherent nucleus scattering. This project will also collect data during the 2022 Los Alamos Neutron Science Center (LANSCE) beam cycle for high statistics measurements of the coherent neutrino interaction rate in argon and an improved search for low mass dark matter. Both measurement are high impact and would advance the field of particle physics. Other benefits include measuring charge current neutrino scattering cross sections important for Deep Underground Neutrino Experiment (DUNE) supernova measurements, and operation and calibration of photomultiplier tube photon detection systems in a large liquid argon detector where scintillation light absorption is a challenge.

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Posters

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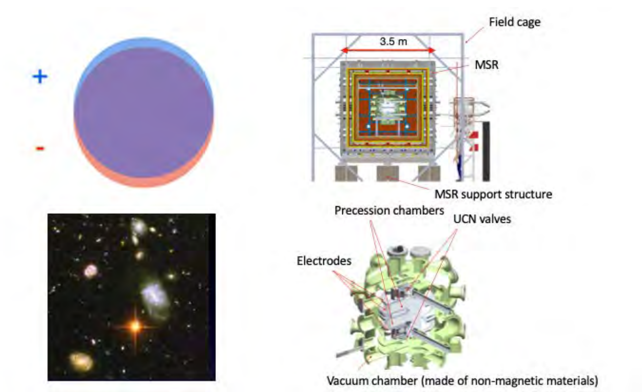
**Peer-reviewed*

The Neutron Electric Dipole Moment as a Gateway to New Physics

Takeyasu Ito
20190041DR



The electric dipole moment (EDM) measures the separation of positive and negative charges inside a subatomic system. Measuring the EDM of the neutron (nEDM) will provide a clue to the puzzle of why there is so much matter than antimatter in this Universe. This LDRD funded project develops a capability to measure the nEDM with an unprecedented sensitivity and theoretical tools to provide a precise interpretation of the experimental results.

Project Description

The research supported by this project addresses the question "Why does the Universe that we live in have so much more matter than antimatter", one of the biggest questions in present day science. This project, on completion, will have demonstrated a capability to perform next generation experiments looking for neutron electric dipole moment, have controlled systematics important for all such experiments, and have developed a theory to use results from these experiments to constrain theories of new physics. Collectively, this research will have a profound impact on our understanding of the interaction among the fundamental building blocks of our world and the history of the Universe. The methods of precision measurements and computation will benefit other researches performed at the Laboratory and elsewhere. The theory employs the tools of Lattice Quantum ChromoDynamics, which have consistently driven the development of novel computer architectures for a long time. The theoretical work done as part of this project will not only enhance the laboratory's stature among theoretical physicists, thus benefiting in hire and retention of personnel, but will also develop and maintain the capability of employing high performance computing architectures in service of simulating challenging scientific problems.

Technical Outcomes

This project achieved the goals of connecting experimental constraints with physics beyond the Standard Model. The calculational side of the project uncovered previously unknown systematics, and studied methods to solve these. The experimental part of the project made significant progress towards the original goal of building a measurement apparatus and collecting data.

Publications

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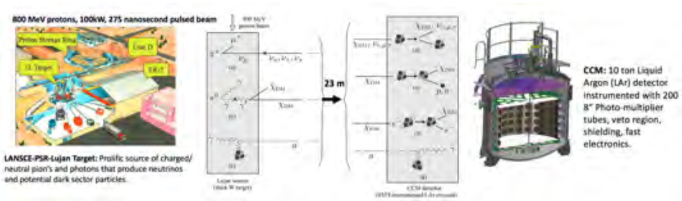
**Peer-reviewed*

Convincing Search for Sterile Neutrinos at Lujan

Richard Van De Water
20190098DR



The Coherent CAPTAIN-Mills (CCM) experiment will search for sterile neutrinos and dark sector particles at the Los Alamos Neutron Science Center (LANSCE) Lujan center. The LANSCE accelerator directs an intense proton beam on a tungsten target that generates neutrinos and possible dark sector particles that can be detected by the sensitive liquid argon CCM detector 23 meters away. This will probe for new physics such as sterile neutrinos and dark sector particles that can account for the missing matter in the Universe. Such a discovery would be revolutionary and stimulate new theories on the origins and evolution of the Universe.

Project Description

This project will have a significant impact on the Laboratory, as it brings experimental neutrino physics back to the place it started in the 1950's with the Nobel Prize winning discovery of the neutrino by Cowen and Reines. High profile Research & Development attracts the brightest and best students, with most of our postdocs going on to successful careers at Los Alamos and at other national labs and universities. We are developing a significant external collaboration of world leading researchers in neutrino physics, who will bring talented students and postdocs to work on the experiment. Fermi National Accelerator Laboratory (FNAL) has expressed support for the project and is allowing a staff scientist to participate. The long-term goal is to develop a robust and flexible neutrino facility to attract new National Science Foundation/Department of Energy (DOE) basic science funding to support novel neutrino experiments and to test technologies for future short- and long-baseline programs. These element are all important to Los Alamos for producing a stronger scientific base, and hence by extension, to DOE/National Nuclear Security Administration, and the nation.

Technical Outcomes

The three main goals of the project were to: 1) build the Coherent Captain-Mills detector; 2) take beam data, perform a sensitive search for dark matter, and publish the results; 3) commission the liquid argon filtration system to improve light output. The first two goals were met, and the third goal almost completed. Long term outcomes will be to use follow-on-funding to search for coherent neutrinos and dark sector particles.

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**Peer-reviewed*

A New Era of Nuclear Physics at the Electron-Ion Collider

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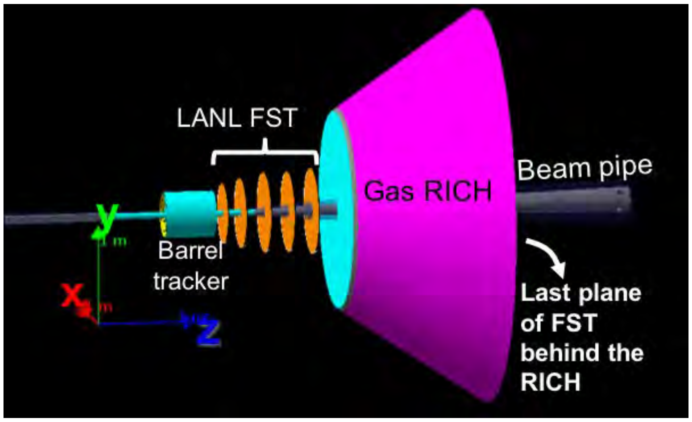
20200022DR



LANL Forward Silicon Tracker (FST), designed as a part of the LDRD project, is representative of our efforts toward major involvement at the future electron-ion collider (EIC). The FST with the proposed silicon technologies illustrates the science we pursue since it is the essential subsystem for the measurement of heavy flavor production at the EIC in the forward proton/nucleus going direction. This design has been characterized in fast and full simulation and the LDRD project developed the related theory that shows how heavy flavor measurements with the FST will shed light on the physics of hadronization.

Project Description

A United States-based high-intensity Electron Ion Collider (EIC) can uniquely address profound questions about nucleons - neutrons and protons - and how they are assembled to from the nuclei of atoms. The EIC will provide the ultimate microscope to determine both the static properties of nucleons and nuclei, as well as how matter and energy can be transported through a strongly interacting quantum mechanical environment. The production and propagation of long-lived heavy subatomic particles is a unique and critical part of this planned decade-long research program. The EIC is an essential component of the Department of Energy's mission to understand all forms of nuclear matter, and this project will enable the use of jets of heavy particles to accomplish this task. It will ensure that the United States maintains its leadership in state-of-the art detector technology, high performance and quantum computing. A secondary long-term benefit from the project is high-resolution, ultra-fast, radiation hard silicon technology that can find applications in dynamic experiments that help certify our nuclear stockpile. Current and future experimental imaging efforts using existing light sources such as the Linac Coherent Light Source and the Advanced Photon Source can also benefit from faster imaging detectors.

Technical Outcomes

This successful project places Los Alamos as a leader in Electron Ion Collider science. The team leveraged unique theory capabilities and flagship silicon tracking expertise to develop the theory of particle and jet production in electron-nucleus collisions, and to define the physics and design of the silicon tracking detector subsystem. In addition, this combined theoretical and experimental effort resulted in important advances in high performance and quantum computing with applications to nuclear physics.

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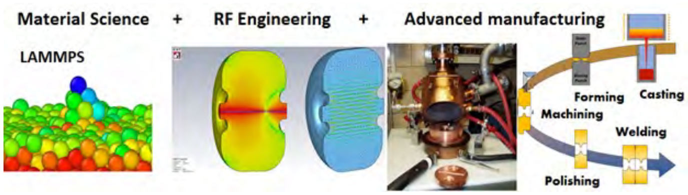
**Peer-reviewed*

High-Gradient, High-Efficiency Radio-Frequency (RF) Structures: Smart Design Based on Informed Break-Down Suppression

Evgenya Simakov
20200057DR



This project uses a multidisciplinary approach to develop ultra-high gradient, efficient RF-structures for particle acceleration. The project team will use molecular dynamics simulations to optimize materials for structure fabrication and high gradient performance. RF and beam physics simulations are used to optimize structure's geometry. The team will employ advanced manufacturing methods to produce better performing structures and manufacture structures of new materials..

Project Description

Particle accelerators are established tools for solving national security challenges, as well as for discovery science. Current missions with national security implications include the need to study and develop materials under extreme conditions that never have been accessible before, higher energy accelerators for proton radiography for stockpile stewardship, and improved tools for remote sensing in defense from national security threats. These represent the range of accelerator systems from large to small. The tools and technologies developed in this project will enable follow-on technology development efforts with significant impact on the performance and cost of accelerator systems. Studies on material extremes and proton radiography at increased energies both require large accelerator systems for which new radio-frequency (RF)-structure technology will reduce size (length typically ~ 1000 yards) and complexity, and increase the efficiency of accelerator systems by an order of magnitude.
For remote sensing applications the use of such RF-structures provides a path to trailer-bed mountable mobile systems for detection of special nuclear materials (SNM). Novel design and engineering tools will provide the first ever integrated RF-structure design using custom-designed materials that suppress limiting RF-break-down in high performance operation. The effort will also establish the first United States-based C-band test accelerator site.

Technical Outcomes

This project commissioned the first C-band test accelerator site in the United States, the C-band Engineering Research Facility in New Mexico, using it to conduct high-gradient testing of four accelerating cavities. Superior performance of accelerator cavities made of copper-silver alloys as compared to pure copper cavities was explained through this work. Additionally, a theoretical model was developed explaining coupling between strong electric fields and multiplication of dislocations in the bulk and surface of a material.

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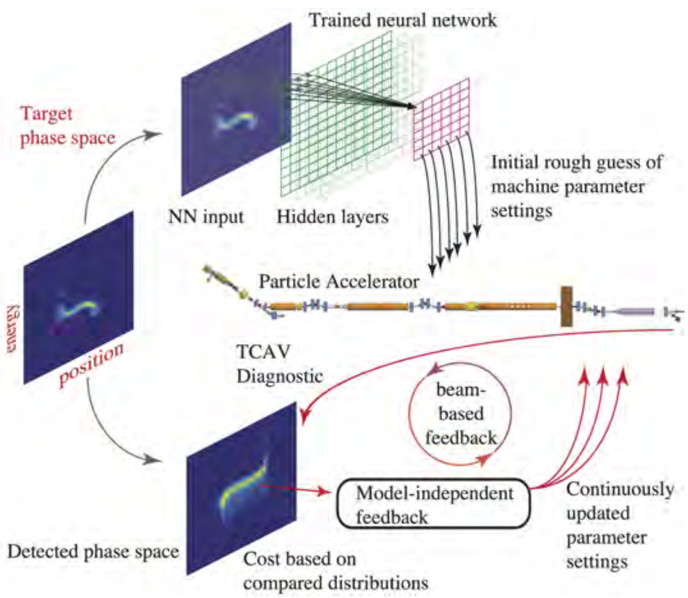
A. Zuboraj, M. R., D. V. Gorelov, T. W. Hall, M. E. Middendorf, D. Rai, E. I. Simakov and T. Tajima. HIGH GRADIENT TESTING OF THE BENCHMARK a/\xce\xbb=0.105 CAVITY AT CERF-NM. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-28190)

A. Zuboraj, M. R., T. W. Hall, D. V. Gorelov, M. E. Middendorf, D. Rai, E. I. Simakov and T. Tajima. HIGH GRADIENT TESTING RESULTS OF THE C-BAND BENCHMARK a/\xce\xbb=0.105 CAVITIES AT LANL. Presented at *Advanced Accelerator Concepts Workshop (AAC)*, Hauppauge, New York, United States, 2022-11-06 - 2022-11-11. (LA-UR-22-31697)

**Peer-reviewed*

Adaptive Machine Learning for Closely Spaced Ultra-Short Intense Accelerator Beams

Alexander Scheinker
20210595DR



An adaptive machine learning setup is shown in which desired two-dimensional longitudinal phase space (z,E) distribution images are used as input to a convolutional neural network (CNN) whose output is a prediction of the accelerator parameters required to achieve the desired distribution. The CNN's output is then adaptively tuned based on local model-independent feedback to make the scheme robust to time variation and noise in the system.

Project Description

Particle accelerators are some of the most useful tools for research because of their ability to probe the interior of subatomic particles, to provide extremely bright and short flashes of X-rays that capture the dynamics of shockwaves, chemical, and biological processes, to produce images of explosion-driven shock wave dynamics in large samples, and for medical isotope production. Accelerators are extremely powerful, large, complex machines with thousands of interconnected components that drift with time and beams that must be tightly focused and precisely accelerated while undergoing complicated nonlinear motion. The main goals of this project are to develop physics-informed adaptive machine learning tools to create controls and diagnostics that improve the performance of all existing accelerators and enable the creation of new machines with beyond state-of-the-art capabilities. In particular, our tools are meant to: 1) decrease the large amounts of wasted time and money in re-tuning after a shut down or to make large parameter changes between various experiments, 2) optimize the current suboptimal performance of operating accelerators by automatically adjusting as beams and accelerator components drift with time, 3) overcome fundamental limitations such as an inability to accelerate trains of closely spaced high intensity charged particle bunches in efficient structures.

Technical Outcomes

The team developed and implemented a model-independent automatic control tool for the Los Alamos Neutron Science Center (LANSCE) accelerator, demonstrated proof-of-concept studies of adaptive machine learning for non-invasive charged particle beam phase space diagnostics, and applied adaptive machine learning methods for automated optimal photocathode growth. The project also developed methods of efficient learning of accurate surrogate models for complex systems.

Publications

Journal Articles

Diaw, A., M. McKerns, I. Sagert, L. G. Stanton and M. S. Murillo. Efficient Learning of Accurate Surrogates for Simulations of Complex Systems. Submitted to *Nature Machine Intelligence*. (LA-UR-20-24947)

*Pavlenko, V., J. Smedley, A. Scheinker, R. L. Fleming, A. Alexander, M. A. Hoffbauer and N. A. Moody. Stoichiometry control and automated growth of alkali antimonide photocathode films by molecular beam deposition. 2022. *Applied Physics Letters*. **120** (9): 91901. (LA-UR-21-30432 DOI: 10.1063/5.0080948)

*Scheinker, A. Adaptive Machine Learning for Robust Diagnostics and Control of Time-Varying Particle Accelerator Components and Beams. 2021. *Information*. **12** (4): 161. (LA-UR-21-24256 DOI: 10.3390/info12040161)

*Scheinker, A. Adaptive machine learning for time-varying systems: low dimensional latent space tuning. 2021. *Journal of Instrumentation*. **16** (10): P10008. (LA-UR-21-26483 DOI: 10.1088/1748-0221/16/10/P10008)

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Conference Papers

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Reports

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Unpublished report. (LA-UR-21-24972)

Presentation Slides

Koglin, J. E., J. E. Coleman, M. McKerns, A. Scheinker and D. T. Wakeford. Machine Learning for Source Optimization at DARHT. Presented at *J32HDT Meeting*, Las Vegas, Nevada, United States, 2023-03-21 - 2023-03-23. (LA-UR-23-22705)

McKerns, M. mystic: physics-informed learning and automated design/control under uncertainty. Presented at *Applied Machine Learning Symposium*, Los Alamos, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-27369)

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Presented at *CAMERA Workshop on Autonomous Discovery in Science and Engineering*, Berkeley, California, United States, 2021-04-20 - 2021-04-22. (LA-UR-21-30257)

Pavlenko, V. Automated growth of photocathode films: from the basics of process control towards artificial intelligence. Presented at *Photocathode Physics for Photoinjectors (P3) Workshop*, Menlo Park, California, United States, 2021-11-10 - 2021-11-12. (LA-UR-21-31176)

Pavlenko, V. Automated Growth of Photocathodes. . (LA-UR-22-20586)

Pavlenko, V. Alkali antimonide cathodes for photoinjectors: Toward reliable fabrication methods. Presented at *LCLS-II-HE Collaboration: Technical Seminar Series*, Menlo Park, California, United States, 2022-04-15 - 2022-04-15. (LA-UR-22-23388)

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Scheinker, A. Adaptive Machine Learning for Time-Varying Systems. Presented at *OWLE seminar at PSI*, Los Alamos, New Mexico, United States, 2021-05-27 - 2021-05-27. (LA-UR-21-24255)

Scheinker, A. Adaptive Machine Learning and Feedback Controls for Particle Accelerators. Presented at *EPICS meeting*, Los Alamos, New Mexico, United States, 2021-07-21 - 2021-07-23. (LA-UR-21-26509)

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Scheinker, A. Adaptive Machine Learning for Control and Virtual Diagnostics of Time-Varying Particle Accelerator Systems and Beams. Presented at *AI for Particle Accelerators, X-ray Beamlines, and Electron Microscopy Workshop @ ANL*, Lemont, Illinois, United States, 2021-11-01 - 2021-11-01. (LA-UR-21-30943)

Scheinker, A. Adaptive Machine Learning for Automatic Control and Non-invasive Diagnostics of Time- Varying Charged Particle Beams. Presented at *ML for accelerators meeting*, Los Alamos, New Mexico, United States, 2021-12-01 - 2021-12-01. (LA-UR-21-31583)

Scheinker, A. Adaptive Machine Learning for Particle Accelerator Tuning. Presented at *Extreme Storage Rings Workshop 2022*, Los Alamos, New Mexico, United States, 2022-01-31 - 2022-01-31. (LA-UR-22-20999)

Scheinker, A. Adaptive tuning of the latent space of encoder-decoder convolutional neural networks for virtual 6D diagnostics of time-varying charged particle beams. Presented at *APS March Meeting 2022*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22659)

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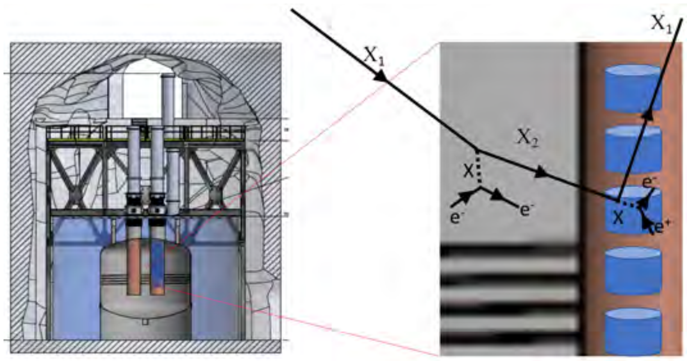
Posters

Koglin, J. E., J. E. Coleman, M. McKerns, D. Ronquillo and A. Scheinker. Progress toward improving accelerator performance and automating operations with advanced analysis software. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-08 - 2022-08-12. (LA-UR-22-27302)

**Peer-reviewed*

Understanding and Development of Germanium (Ge) Detectors to Elucidate the Nature of Dark Matter, the Origin of Neutrino Mass and its Connection to the Matter-Antimatter Asymmetry

Steven Elliott
20220672DR



Left: A concept of the experiment layout of Ge detectors within a liquid argon shield. Right: An example of the type of dark matter event that might become visible with this layout if the proposed R&D is successful in better understanding the detector response and the particle interactions. The example, is of a boosted dark matter particle (X1) producing a heavy dark matter particle (X2) while interacting with an electron and being detected within the argon. The X2 then decays back to X1 producing other detectable particles, here depicted by an electron-positron pair.

Project Description

This project will positively impact Los Alamos National Laboratory programs supported by the Department of Energy Office of Science (DOE-SC) Office of Nuclear Physics and Office of High Energy Physics. The technologies developed will not only impact this basic science effort, but will build capability for radiation detection and potentially impact other laboratory missions.

Technical Outcomes

The project successfully met the goals of designing a detector charge trapping system, upgrading an existing test stand for better light detectors and performing theoretical calculations for double beta decay and dark matter.

Publications

Journal Articles

*Arnquist, I. J., F. T. Avignone, A. S. Barabash, C. J. Barton, K. H. Bhimani, E. Blalock, B. Bos, M. Busch, M. Buuck, T. S. Caldwell, Y. -. D. Chan, C. D. Christofferson, P. -. H. Chu, M. L. Clark, C. Cuesta, J. A. Detwiler, Y. Efremenko, H. Ejiri, S. R. Elliott, G. K. Giovanetti, M. P. Green, J. Gruszko, I. S. Guinn, V. E. Guiseppe, C. R. Haufe, R. Henning, D. H. Aguilar, E. W. Hoppe, A. Hostiuc, M. F. Kidd, I. Kim, R. T. Kouzes, T. E. V. Lannen, A. Li, A. M. Lopez, J. M. Lopez-Castano, E. L. Martin, R. D. Martin, R. Massarczyk, S. J. Meijer, T. K. Oli, G. Othman, L. S. Paudel, W. Pettus, A. W. P. Poon, D. C. Radford, A. L. Reine, K. Rielage, N. W. Ruof, D. C. Schaper, D. Tedeschi, R. L. Varner, S. Vasilyev, J. F. Wilkerson, C. Wiseman, W. Xu, C. -. H. Yu and B. X. Zhu. Search for Solar Axions via Axion-Photon Coupling with the Majorana Demonstrator. 2022. *Physical Review Letters*. **129** (8): 081803. (LA-UR-22-23621 DOI: 10.1103/PhysRevLett.129.081803)

Graesser, M. L., G. Li, M. Ramsey-Musolf, T. Shen and S. Urrutia-Quiroga. Uncovering a chirally suppressed mechanism of neutrinoless double beta decay with LHC searches. Submitted to *Journal of High Energy Physics*. (LA-UR-21-32454)

Massarczyk, R., K. R. Rielage, S. R. Elliott, S. J. Meijer, D. Schaper and I. w. Kim. Charge Trapping and Energy Performance of the Majorana Demonstrator. Submitted to *Physical Review C*. (LA-UR-22-26513)

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Massarczyk, R., S. R. Elliott, D. E. Fields, M. Gold and N. C. Mcfadden. Understanding the enhancement of scintillation light in xenon-doped liquid argon. 2022. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. 167707. (LA-UR-22-23376 DOI: 10.1016/j.nima.2022.167707)

Massarczyk, R., S. R. Elliott, P. Chu, I. w. Kim, K. R. Rielage, S. J. Meijer and D. Schaper. Searches for Atomic Transitions Violating the Pauli Exclusion Principle or Charge Conservation with the Majorana Demonstrator. Submitted to *Physical Review Letters*. (LA-UR-22-23620)

Conference Papers

Elliott, S. R., P. Chu, R. Massarczyk, S. J. Meijer, K. R. Rielage and I. w. Kim. Modeling Backgrounds for the MAJORANA DEMONSTRATOR. Presented at *Low Radioactivity Techniques*. (Rapid City, South Dakota, United States, 2022-06-14 - 2022-06-17). (LA-UR-22-29582)

Reports

Mereghetti, E., V. Cirigliano, Z. Davoudi, W. G. Dekens, J. de Vries, J. Engel, X. Feng, J. Gehrlein, M. L. Graesser, L. Graf, H. Hergert, L. Jin, A. Nicholson, S. Pastore, M. Ramsey-Musolf, M. Spinrath, U. van Kolck and A. Walker-Loud. Neutrinoless double beta decay: a roadmap for matching theory to experiment. Unpublished report. (LA-UR-22-22587)

Presentation Slides

Massarczyk, R., N. Poudyal and W. Xu. Upgrading the BACoN liquid argon cryogenic system to study scintillation light. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Nuclear Physics (DNP)*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-27. (LA-UR-22-31418)

Mereghetti, E. Bridging particle and nuclear physics for neutrinoless double beta decay with EFTs. Presented at *Conference on the Intersections of Nuclear and Particle Physics*, Buena Vista, Florida, United States, 2022-08-29 - 2022-09-04. (LA-UR-22-29217)

Posters

Kim, I. w., S. R. Elliott and R. Massarczyk. Beyond-the-Standard-Model physics searches with LEGEND-1000. Presented at *The XXX International Conference on Neutrino Physics and Astrophysics*, Seoul, Korea, South, 2022-05-30 - 2022-06-04. (LA-UR-22-24307)

Massarczyk, R., S. R. Elliott and N. Poudyal. Upgrading the BACoN liquid argon cryogenic system to study light. Presented at *2022 Conference on Science at Sanford Underground Research Facility*, Rapid City, New Mexico, United States, 2022-05-11 - 2022-05-13. (LA-UR-22-24103)

**Peer-reviewed*

Neutrino Physics with Short-and Long-baseline Experiments

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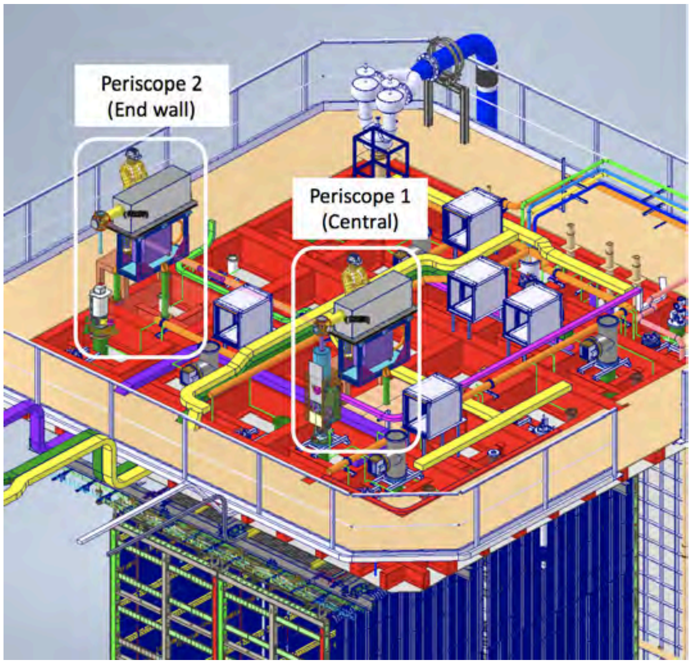

Two Ionization laser calibration system models (as shown in the enclosed white boxes) shown integrated on top of the ProtoDUNE detector at the European Organization for Nuclear Research (CERN) lab in Switzerland. This image signifies the progress made over the past year in developing two full designs of the laser calibration systems along with progress made towards integrating them in ProtoDUNE where they will be installed in early FY2022.

Project Description

Why do we live in a matter-dominated universe? The tiny, subatomic particles called "neutrinos" may hold the answer to this most sought-after question. The Deep Underground Neutrino Experiment (DUNE) which forms the United States flagship experiment aims to explore this by sending neutrinos over 800 miles from Illinois to South Dakota. Several neutrino experiments in the recent past reported anomalous results that indicate there maybe more than three types of neutrinos ("sterile" neutrinos), which if proved to be true will have significant implications to our current understanding of neutrinos. The Short-Baseline Neutrino (SBN) program at Fermilab is exploring existing hints to address this. Both of these efforts are part of the high energy physics mission for Department of Energy (DOE) Office of Science. The proposed research spans the DUNE and SBN experiments and significantly enhances their technical and physics capabilities towards achieving the above stated goals. Novel calibration techniques using a high-power laser system and a source of low energy neutral particles ("neutrons") are proposed in order to achieve the measurement precision needed for DUNE. At SBN, a rare particle production process will be studied to address the sterile neutrino question which will be a "breakthrough" result in neutrino physics.

Publications

Journal Articles

*Abi, B., R. Acciarri, M. A. Acero, G. Adamov, D. Adams, M. Adinolfi, Z. Ahmad, J. Ahmed, T. Alion, S. A. Monsalve, C. Alt, J. Anderson, C. Andreopoulos, M. P. Andrews, F. Andrianala, S. Andringa, A. Ankowski, M. Antonova, S. Antusch, A. Aranda-Fernandez, A. Ariga, L. O. Arnold, M. A. Arroyave, J. Asaadi, A. Aurisano, V. Aushev, D. Autiero, F. Azfar, H. Back, J. J. Back, C. Backhouse, P. Baesso, L. Bagby, R. Bajou, S. Balasubramanian, P. Baldi, B. Bambah, F. Barao, G. Barenboim, G. J. Barker, W. Barkhouse, C. Barnes, G. Barr, J. B. Monarca, N. Barros, J. L. Barrow, A. Bashyal, V. Basque, F. Bay, J. L. B. Alba, J. F. Beacom, E. Bechetoille, B. Behera, L. Bellantoni, G. Bellettini, V. Bellini, O. Beltramello, D. Belver, N. Benekos, F. B. Neves, J. Berger, S. Berkman, P. Bernardini, R. M. Berner, H. Berns, S. Bertolucci, M. Betancourt, Y. Bezawada, M. Bhattacharjee, B. Bhuyan, S. Biagi, J. Bian, M. Biassoni, K. Biery, B. Bilki, M. Bishai, A. Bitadze, A. Blake, B. B. Siffert, F. D. M. 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Coelho, E. Conley, J. M. Conrad, M. Convery, L. Corwin, P. Cotte, L. Cremaldi, L. Cremonesi, J. I. Crespo-Anad\xc3\xb3n, E. Cristaldo, R. Cross, C. Cuesta, Y. Cui, D. Cussans, M. Dabrowski, H. d. Motta, L. Da Silva Peres, C. David, Q. David, G. S. Davies, S. Davini, J. Dawson, K. De, R. M. De Almeida, P. Debbins, I. De Bonis, M. P. Decowski, A. de Gouv\xc3\xaaa, P. C. De Holanda, I. L. De Icaza Astiz, A. Deisting, P. De Jong, A. Delbart, D. Delepine, M. Delgado, A. Dell'Acqua, P. De Lurgio, J. R. T. de Mello Neto, D. M. DeMuth, S. Dennis, C. Densham, G. Deptuch, A. De Roeck, V. De Romeri, J. J. De Vries, R. Dharmapalan, M. Dias, F. Diaz, J. S. D\xc3\xadaz, S. D. Domizio, L. D. Giulio, P. Ding, L. D. Noto, C. Distefano, R. Diurba, M. Diwan, Z. Djurcic, N. Dokania, M. J. Dolinski, L. Domine, D. Douglas, F. Drielsma, D. Duchesneau, K. Duffy, P. Dunne, T. Durkin, H. Duyang, O. Dvornikov, D. A. Dwyer, A. S. Dyshkant, M. Eads, D. Edmunds, J. Eisch, S. Emery, A. Ereditato, C. O. Escobar, L. 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Gollapinni, S. and N. P. Oza. Measuring the Neutral Current \xcf \x800 Cross-section on Argon in MicroBooNE. Presented at *Fermilab Annual Users' Meeeting 2022*, Batavia, Illinois, United States, 2022-06-13 - 2022-06-16. (LA-UR-22-25423)

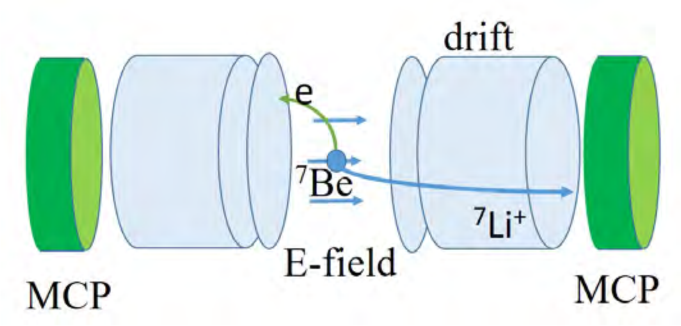
Mogan, A., S. Gollapinni and MicroBooNE Collaboration. Constraining the Neutral Current Pi0 Background for MicroBooNE's Single-Photon Search. Presented at *XXIX INTERNATIONAL CONFERENCE ON NEUTRINO PHYSICS*

(Neutrino 2020), Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28826)

**Peer-reviewed*

Laser Cooling and Trapping Beryllium

Xinxin Zhao
20210044ER



Electron and recoil ion detection illustration (conceptual design). Electron and recoil ion are extracted and guided onto MCP detectors, their position and time of flight (TOF) will be used for energy and momentum reconstruction of beryllium-7 (Be-7) electron capture decay

Project Description

The ability to laser cool and trap beryllium isotopes has exciting applications involving both the Los Alamos National Laboratory (LANL) nuclear forensics mission and fundamental science. For the LANL nuclear forensics mission, the beryllium 10 (Be-10) isotope can be used to reveal information about the carbon mass of a nuclear device. In fundamental science, Be-7 radioisotopes can be used to probe the existence of kiloelectron volt (keV)-mass sterile neutrinos with unprecedented sensitivity. Discovery of sterile neutrinos will have profound implications on three of the most urgent open problems in physics: the nature of neutrino masses, the nature of dark matter, and the origin of the matter-antimatter asymmetry in the universe. The common challenge in both emerging applications is trapping neutral Be atoms, and we propose to demonstrate the first Magneto-Optical Trapping of Be atoms to solve it.

Publications

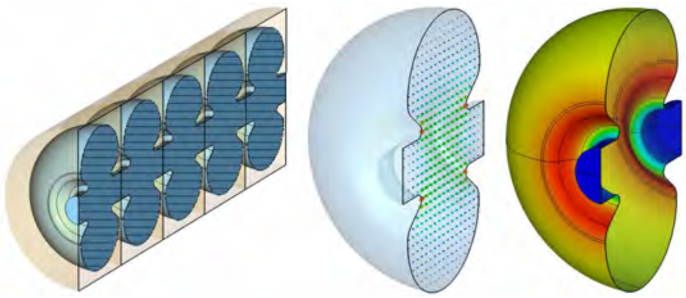
Presentation Slides

Ahrens, J. P. LDRD ISTI Proposal Review (20210527CR) Information Science and Technology Institute (ISTI): Foundational Research in Information Science and Technology. . (LA-UR-20-28422)

**Peer-reviewed*

Compact High-Gradient Booster for Enhanced Proton Radiography

Sergey Kurennoy
20210048ER



High-gradient S-band structure operating at 2817.5 megahertz (MHz) for beam velocity v/c=0.84 (left to right): 5-cell structure section; electric field within a cell; current distribution on the cell inner surface. Such structures can support very high accelerating gradients to accelerate beams within short distances. Our proposed high-gradient booster at LANSCE will consist of similar structures at three different frequencies. It will accelerate protons, delivered by the existing 800-meters-long linac, from 800 million electronvolt (MeV) to 3 giga-electronvolt (GeV) within tens of meters to increase the proton radiography resolution by an order of magnitude.

Project Description

Our project aims to develop a compact linear accelerator (< 50 meter) to boost the beam energy of protons at Los Alamos Neutron Science Center (LANSCE) from 0.8 gigaelectronvolt (GeV), provided by the existing accelerator, to 3 GeV. This energy increase will improve the proton radiography resolution 10 times. The compact booster will be based on high-gradient cavities that we will adapt for proton beams. This enhancement of proton radiography capability at LANSCE, which can be accomplished without significant changes to the existing infrastructure, will benefit National Nuclear Security Administration Defense Programs and fundamental materials research. High-gradient structures potentially can provide compact proton accelerators for cancer therapy and homeland defense.

Publications

Journal Articles

Batygin, Y. K. Beam dynamics in independent phased cavities. 2022. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **1040**: 167192. (LA-UR-22-25550 DOI: 10.1016/j.nima.2022.167192)

Conference Papers

Batygin, Y. K. Longitudinal Beam Dynamics in Array of Equidistant Multicell Cavities. Presented at *International Linear Accelerator Conference 2022 (LINAC2022)*. (Liverpool, United Kingdom, 2022-08-28 - 2022-09-02). (LA-UR-22-28774)

Batygin, Y. K. and S. S. Kurennoy. Design of 3-GeV High-Gradient Booster for Upgraded Proton Radiography at LANSCE. Presented at *North American Particle Accelerator Conference (NAPAC)*. (Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12). (LA-UR-22-27594)

Batygin, Y. K. and S. S. Kurennoy. High-Gradient 3-GeV Booster for Enhanced Proton Radiography at LANSCE. Presented at *20th Advanced Accelerator Concepts Workshop (AAC'22)*. (Hauppauge, New York, United States, 2022-11-06 - 2022-11-11). (LA-UR-23-20984)

Kurennoy, S. S., Y. K. Batygin and E. R. Olivas. Accelerating Structures for High-Gradient Proton Radiography Booster at LANSCE. Presented at *North American Particle Accelerator Conference (NAPAC)*. (Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12). (LA-UR-22-27859)

Kurennoy, S. S., Y. K. Batygin and E. R. Olivas. Development of High-Gradient Accelerating Structures for Proton Radiography Booster at LANSCE. Presented at *Linear Accelerator Conference (LINAC)*. (Liverpool, United Kingdom, 2022-08-28 - 2022-09-02). (LA-UR-22-28838)

Kurennoy, S. S., Y. K. Batygin and E. R. Olivas. High-Gradient Accelerating Structures for 3-GeV Proton Radiography Booster. Presented at *Advanced Accelerator Concepts Workshop (AAC)*. (Long Island, New York, United States, 2022-11-06 - 2022-11-11). (LA-UR-23-20597)

Kurennoy, S. S. and Y. K. Batygin. High-Gradient Booster for Enhanced Proton Radiography at LANSCE. Presented at *12th International Particle Accelerator Conference - IPAC'21(virtual)*. (Campinas, Brazil, 2021-05-24 - 2021-05-28). (LA-UR-21-24609)

Presentation Slides

Batygin, Y. K. and S. S. Kurennoy. Progress in Design of 3-GeV High-Gradient pRad Booster for LANSCE. Presented at *LANSCE Futures Spring 2021 Workshop Series: Dynamic Radiography*, Los Alamos (virtual format), New Mexico, United States, 2021-04-05 - 2021-04-06. (LA-UR-21-23157)

Batygin, Y. K. and S. S. Kurennoy. Design of 3-GeV High-Gradient Booster for Upgraded Proton Radiography at LANSCE. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-27874)

Batygin, Y. K. and S. S. Kurennoy. High-Gradient 3-GeV Booster for Enhanced Proton Radiography at LANSCE. Presented at *20th Advanced Accelerator Concepts Workshop (AAC'22)*, Hauppauge, New York, United States, 2022-11-06 - 2022-11-11. (LA-UR-22-31608)

Batygin, Y. K. and S. S. Kurennoy. Design of 3 GeV High-Gradient Booster for Upgraded Proton Radiography at LANSCE. Presented at *Los Alamos National Laboratory Engineering Week*, Los Alamos, New Mexico, United States, 2023-02-22 - 2023-02-23. (LA-UR-23-21310)

Kurennoy, S. S., Y. K. Batygin and E. R. Olivas. Accelerating Structures for High-Gradient Proton Radiography Booster at LANSCE. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-28189)

Kurennoy, S. S., Y. K. Batygin and E. R. Olivas. High-Gradient Accelerating Structures for 3-GeV Proton Radiography Booster. Presented at *Advanced Accelerator Concepts Workshop (AAC)*, Long Island, New York, United States, 2022-11-06 - 2022-11-11. (LA-UR-22-31724)

Kurennoy, S. S. and R. D. Ryne. Parallel Simulation of Beam Dynamics in Particle Accelerators. . (LA-UR-23-23332)

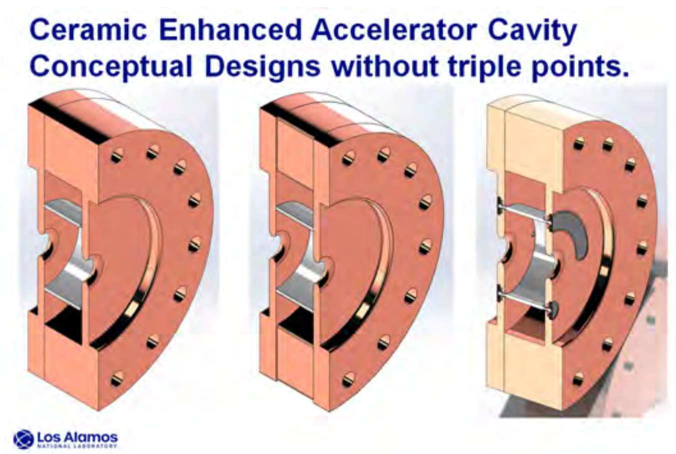
Posters

Batygin, Y. K. Longitudinal Beam Dynamics in Array of Equidistant Multicell Cavities. Presented at *International Linear Accelerator Conference 2022 (LINAC2022)*, Liverpool, United Kingdom, 2022-08-28 - 2022-09-02. (LA-UR-22-28705)

**Peer-reviewed*

Ceramic Enhanced Accelerator Structures

Leanne Duffy
20210083ER



Ceramic enhanced accelerator cavities have the potential to improve the radio frequency (RF) efficiency of normal conducting accelerator cavities by 40%. Here we present some initial concepts of cavity designs that eliminate problematic triple-points (locations of three materials meeting that have high field enhancement). The ceramic rings in the cavities essentially add more space and significantly reduce the field in the outer radial region, decreasing the RF wall losses.

Project Description

Pillbox accelerator cavities are used everywhere because they are inexpensive, reliable, work over a huge frequency range, and accelerate electron beams as well as proton and ion beams. Our innovative new cavity designs will increase efficiency by 40% over normal conducting accelerator cavities without compromising performance criteria. This technology will also improve delivery of high-brightness electron beams, a crucial improvement for next generation large-scale accelerator projects such as x-ray light sources and linear colliders. Upgraded linac structures for the Los Alamos Neutron Science Center (LANSCE) will be of interest to the National Nuclear Security Administration as a risk mitigation and capability enhancement strategy. Development of intrinsically wake-damped, high-efficiency structures is expected to be of high interest to High Energy Physics and Basic Energy Sciences within Department of Energy-Office of Science, via direct impact to the length and power consumption, and therefore cost, of next-generation research and user facility accelerators.

Publications

Journal Articles

*Upadhyay, J., H. Xu, K. Nichols and J. W. Lewellen. Design of a ceramic enhanced normal conducting standing wave accelerator structure for higher shunt impedance. 2022. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **1034**: 166669. (LA-UR-20-25095 DOI: 10.1016/j.nima.2022.166669)

Conference Papers

Xu, H., M. R. Bradley, M. A. Holloway, J. Upadhyay and L. D. Duffy. Ceramic enhanced accelerator structure low power test and designs of high power and beam tests. Presented at *North American Particle Accelerator Conference (NAPAC)*. (Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12). (LA-UR-22-27134)

Presentation Slides

Nichols, K., J. W. I. Lewellen, L. D. Duffy, M. A. Holloway, E. I. Simakov, J. Upadhyay and F. L. Krawczyk. Employing High Epsilon Dielectric Materials for Enhancing Cu Accelerator. Presented at *Snowmass miniWorkshop on Innovative Design*, Chicago, Illinois, United States, 2021-01-26 - 2021-01-26. (LA-UR-21-20673)

Xu, H., M. R. Bradley, L. D. Duffy, M. A. Holloway and J. Upadhyay. Ceramic enhanced accelerator structure low power test and designs of high power and beam tests. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-27896)

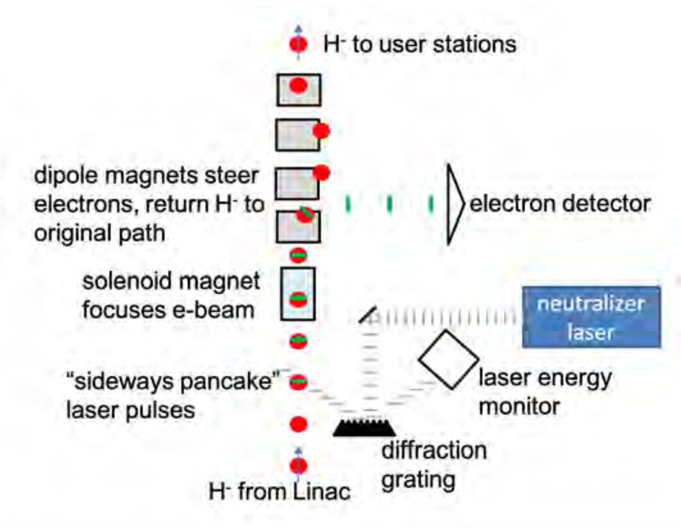
Posters

Bradley, M. R. Ceramic Enhanced Accelerator Space Readiness. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-27283)

**Peer-reviewed*

Neutralizer-Based Longitudinal Bunch Profile Measurement

Heather Andrews
20210156ER



Particle beam "tails" or "halo" are a serious problem for high-power accelerators such as Los Alamos Neutron Science Center (LANSCE). The project team is developing a non-invasive diagnostic to examine these using a high-energy laser to strip electrons off of the H- beam. Magnets after the laser interaction point direct the electrons to a detector and return the hydrogen (H)-beam to its original path. The distribution of detected electrons reflects the distribution of H- particles in a small cross section of the bunch. Scanning the laser along the length of the bunch maps the bunch shape.

Project Description

High-power particle accelerators are foundational tools used to support missions that address national security challenges, in particular stockpile stewardship. This work addresses two related challenges associated with such accelerators: making high-resolution measurements of the accelerator's particle beam properties while it is in operation; and diagnosing conditions that can result in beam loss inside, and subsequent damage to, the accelerator. Such machines are also useful for basic science research, particularly in nuclear and high-energy physics, where they serve as neutrino factories, spallation neutron sources, exotic beam drivers, etc.; this work will help address the operating challenges of all such machines.

Publications

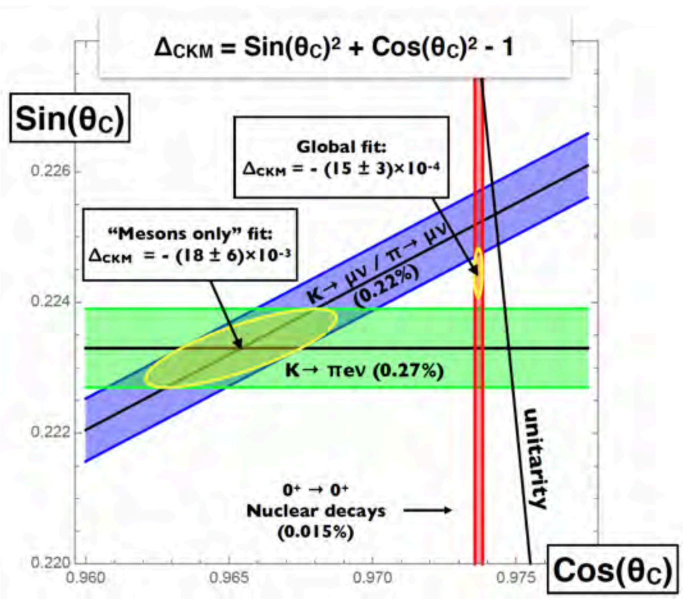
Posters

Andrews, H. L., J. L. Medina, C. G. Miera, R. T. Thornton and C. E. Taylor. A Laser-Neutralization Based Bunch Length Diagnostic for LANSCE. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-27871)

**Peer-reviewed*

Deconstructing the Cabibbo Angle Anomaly

Emanuele Mereghetti
20210190ER



Universality of the weak interactions in the Standard Model requires that down- and strange-quarks share the Fermi constant in proportion to the cosine and sine of the Cabibbo angle. Recent developments show a 3-5 standard deviation tension. Using effective field theory methods, this project addresses three main challenges: (i) the robustness of the theoretical uncertainties (thickness of the bands); (ii) the impact of ongoing and future precision measurements of neutron decay at the LANL Ultra Cold Neutron facility; (iii) what new interactions could shift the bands around so that they meet in one point lying on the unitarity circle.

Project Description

This project will develop the theoretical and computational tools needed to probe the fundamental constituents of matter and their interactions through precision measurements of neutron and nuclear beta disintegrations. This project is very timely due to the recent emergence of tensions between measurements and the interpretation in terms of the known physical laws governing subatomic physics. The project goal is to improve the theoretical precision of beta disintegrations of nuclei and thus assess the possibility that new phenomena might impact them. Furthering the understanding of matters constituents and interactions and possibly discovering new ones is a significant component of the Department of Energy (DOE) Office of Science (Nuclear Physics) mission, as elucidated in the latest Long Range Plan by the Nuclear Science Advisory Committee. The success of this project would have a strong positive impact on the Los Alamos and broader DOE experimental program in precision beta decay studies.

Publications

Journal Articles

Cirigliano, V., D. Bryman, A. Crivellin and G. Inguglia. Testing Lepton Flavor Universality Violation in the Charged Current with Kaon, Pion, Tau and Beta Decays. Submitted to *Annual Review of Nuclear and Particle Science*. (LA-UR-21-30608)

*Cirigliano, V., D. Diaz-Calderon, A. Falkowski, M. Gonzalez-Alonso and A. Rodriguez-Sanchez. Semileptonic tau decays beyond the Standard Model. 2022. *Journal of High Energy Physics*. **2022** (4): 152. (LA-UR-21-31791 DOI: 10.1007/JHEP04(2022)152)

Cirigliano, V., E. Mereghetti, L. M. Hayen, A. Walker-Loud and J. de Vries. Radiative correction to neutron decay in effective field theory. Submitted to *Physical Review Letters*. (LA-UR-21-31960)

*Cirigliano, V., W. Dekens, J. De Vries, M. Hoferichter and E. Mereghetti. Toward Complete Leading-Order Predictions for Neutrinoless Double \xce\xb2 Decay. 2021. *Physical Review Letters*. **126** (17): 172002. (LA-UR-20-30355 DOI: 10.1103/PhysRevLett.126.172002)

*Cirigliano, V., W. Dekens, J. de Vries, K. Fuyuto, E. Mereghetti and R. Ruiz. Leptonic anomalous magnetic moments in ν SMEFT. 2021. *Journal of High Energy Physics*. **2021** (8): 103. (LA-UR-21-24456 DOI: 10.1007/JHEP08(2021)103)

Mereghetti, E., G. King, A. Baroni, V. Cirigliano, S. Gandolfi, L. Hayen, S. Pastore and M. Piarulli. Ab initio calculation of the beta decay spectrum of 6He. Submitted to *Physical Review C*. (LA-UR-21-31938)

Mereghetti, E., R. Boughezal and F. Petriello. Dilepton production in the SMEFT at O(1/Lambda^4). Submitted to *Journal of High Energy Physics*. (LA-UR-21-25379)

Mereghetti, E., V. Cirigliano, W. Dekens, J. de Vries and T. Tong. Beta-decay implications for the W-boson mass anomaly. 2022. *Physical Review D*. **106** (7): 075001. (LA-UR-22-23870 DOI: 10.1103/PhysRevD.106.075001)

Tomalak, O. S., A. Afanasev, A. Schmidt , J. Bernauer , E. Cline, F. Hagelstein, V. Sharkovska, E. Tomasi-Gustafsson, F. Myhrer and P. Blunden. Two-photon exchange in lepton-proton scattering. Submitted to *European Physical Journal A. Hadrons and Nuclei*. (LA-UR-22-32680)

Tomalak, O. S., R. Petti and R. J. Hill. Nucleon axial radius and form factor with future neutrino experiments. Submitted to *discussed upon completion, PRD or PRC are among the options*. (LA-UR-22-32611)

*Tomalak, O., Q. Chen, R. J. Hill and K. S. McFarland. QED radiative corrections for accelerator neutrinos. 2022. *Nature Communications*. **13** (1): 5286. (LA-UR-21-27844 DOI: 10.1038/s41467-022-32974-x)

Reports

Ito, T., E. Mereghetti, S. Clayton, T. Bhattacharya, R. Gupta, K. Fuyuto, C. M. O'Shaughnessy, C. Morris, N. S. Phan, D. Schaper, Z. Tang, S. Baessler, L. Broussard, T. Chupp, B. W. Filippone, L. Hayen, C. Liu, H. P. Mumm, C. Seng, W. M. Snow and A. Young. Fundamental Neutron Physics: a white paper on prospects in the US. Unpublished report. (LA-UR-22-32363)

Tomalak, O. S. Neutrino Scattering Measurements on Hydrogen and Deuterium: A Snowmass White Paper. Unpublished report. (LA-UR-21-31459)

Presentation Slides

Cirigliano, V. and E. Mereghetti. Deconstructing the Cabibbo angle anomaly. . (LA-UR-21-31961)

Delzanno, F. Charged Lepton Flavor Violation at the future Electron-Ion Collider. Presented at *T-Division Lightning Talks*, Los Alamos, New Mexico, United States, 2022-08-09 - 2022-08-10. (LA-UR-22-28198)

Fuyuto, K. Searches for violations of fundamental symmetries. . (LA-UR-22-20417)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-20967)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22082)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22446)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22469)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22561)

Fuyuto, K. Searching for new physics in CP violation. . (LA-UR-22-23320)

Fuyuto, K. Unraveling the origin of neutrino mass. . (LA-UR-22-28333)

Koglin, J. E., J. E. Coleman, M. McKerns, A. Scheinker and D. T. Wakeford. Machine Learning for Source Optimization at DARHT. Presented at *J32HDT Meeting*, Las Vegas, Nevada, United States, 2023-03-21 - 2023-03-23. (LA-UR-23-22705)

Mereghetti, E. Effective Field Theories for BSM searches at low- and high-energy. Presented at *Conference on the Intersections of Particle and Nuclear Physics*, Buena Vista, Florida, United States, 2022-08-29 - 2022-09-04. (LA-UR-22-29216)

Mereghetti, E. Fundamental Symmetries with Nucleons and Nuclei. Presented at *Computational Nuclear Physics and AI/ML workshop*, Washington, District Of Columbia, United States, 2022-09-06 - 2022-09-07. (LA-UR-22-29218)

Tomalak, O. S. Axial and pseudoscalar form factors from charged-current neutrino-nucleon elastic scattering. Presented at *2021 Fall Meeting of the APS DNP, virtual*,

Boston, Massachusetts, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-29985)

Tomalak, O. S. An Overview of Cross Sections in Neutrino Physics. Presented at *14th Conference on the Intersections of Particle and Nuclear Physics (CIPANP 2022)*, Orlando, Florida, United States, 2022-08-29 - 2022-09-04. (LA-UR-22-28913)

Tomalak, O. S. Radiative corrections to neutron beta decay from low-energy effective field theory. Presented at *The 2022 International Conference on the Structure of Baryons, Baryons-2022*, Sevilla, Spain, 2022-11-07 - 2022-11-11. (LA-UR-22-31609)

Tomalak, O. S. Radiative corrections to neutron beta decay from low-energy effective field theory. Presented at *The 2022 International Conference on the Structure of Baryons, Baryons-2022*, Sevilla, Spain, 2022-11-07 - 2022-11-11. (LA-UR-23-20003)

Tomalak, O. S. Radiative corrections in neutrino physics. Presented at *S@INT Seminar Series*, Seattle, Washington, United States, 2023-01-19 - 2023-01-19. (LA-UR-23-20009)

Tomalak, O. S. Radiative corrections for precise low- and high-energy (anti)neutrino flux constraints. Presented at *DIS 2023*, East Lansing, Michigan, United States, 2023-03-29 - 2023-03-31. (LA-UR-23-22298)

Tomalak, O. S. Status of proton radius puzzle and QED radiative corrections for accelerator neutrinos. Presented at *Seminar at KIAS*, Seoul, Korea, South, 2023-04-05 - 2023-04-14. (LA-UR-23-22299)

Tomalak, O. S. QED radiative corrections for accelerator neutrinos. Presented at *Seminar at Institute for Nuclear Physics, Mainz, Germany*, Mainz, Germany, 2023-03-20 - 2023-03-21. (LA-UR-23-22296)

Tomalak, O. S. Radiative corrections to low-energy neutral-current neutrino scattering and DAR sources. Presented at *The Magnificent CEvNS 2023 Workshop*, Munich, Germany, 2023-03-22 - 2023-03-23. (LA-UR-23-22297)

Tomalak, O. S. QED radiative corrections for accelerator neutrinos.. Presented at *XXth Workshop of Soft Collinear Effective Theory*, Berkeley, California, United States, 2023-03-27 - 2023-03-31. (LA-UR-23-23037)

Tomalak, O. S. Radiative corrections in electron and neutrino physics. Presented at *Seminar at JLab Theory Center*, Newport News, Virginia, United States, 2023-04-05 - 2023-04-05. (LA-UR-23-23044)

Tomalak, O. S. Theory and experiment for precision neutrino physics. Presented at *Physics Colloquium at Old Dominion University*, Norfolk, Virginia, United States, 2023-04-06 - 2023-04-06. (LA-UR-23-23048)

Tomalak, O. S. Radiative corrections to low-energy neutral-current neutrino scattering and DAR sources. Presented at *Interplay of Nuclear, Neutrino and BSM Physics at Low-Energies"*, Seattle, Washington, United States, 2023-04-17 - 2023-04-21. (LA-UR-23-23047)

Posters

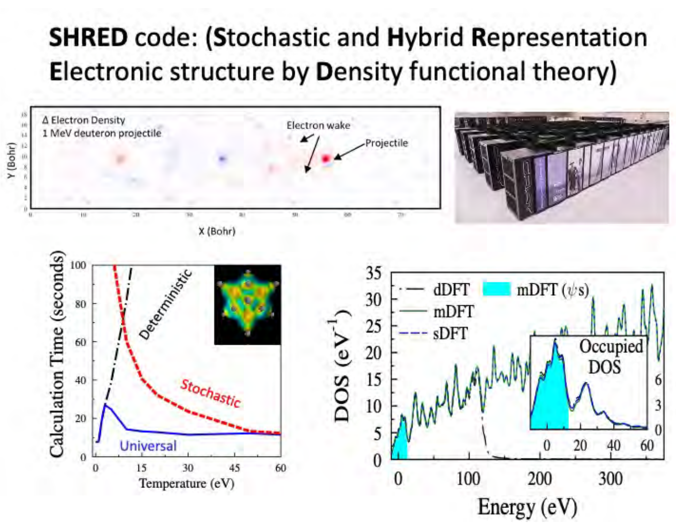
Delzanno, F. Charged Lepton Flavor Violation in High Energy Electron-Proton Scattering. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27297)

Tomalak, O. S. QED corrections to charged-current neutrino-nucleon elastic scattering. Presented at *PANIC 2021: Particles and Nuclei International Conference*, Lisbon, Portugal, 2021-08-05 - 2021-08-10. (LA-UR-21-28153)

**Peer-reviewed*

From Solids to Plasmas: A Universal Approach to Ab Initio Modeling Across Temperature Regimes

Alexander White
20210233ER



Traditional methods for calculating material properties of warm dense matter (WDM) scale poorly with system temperature and number of processors. A novel universal (hybrid representation) approach, based on decomposition of the system's density of states into stochastic and deterministic components (bottom right) provides an efficient algorithm for Kohn Sham density functional theory. The approach scale well on high performance computers (top right) and have improved scaling with temperature (bottom left). Our new code will be used to accurately calculate properties such as electronic stopping power (to right) and equation of state for previously inaccessible WDM conditions.

Project Description

Predictive modeling is critical for understanding complex systems under extreme conditions, where experimental results can be expensive to obtain or difficult to interpret. Successfully modeling such systems requires accurate calculation of material properties, such as equation of state, mass transport and conductivity. Kohn Sham Density Functional Theory (KS-DFT), based on first-principle quantum mechanics, has become the premier method for the calculation of these properties. However, for extreme conditions, these predictive calculations are often numerically intractable. This is because the computational costs of these calculations grow with both temperature and system size. This necessitates a patchwork of more approximate methods for different regimes and often leads to inconsistent results. Our novel approach is based on the unification of the traditional deterministic algorithm for KS-DFT with a recently developed stochastic algorithm to achieve the same accuracy at lower costs. This universal DFT algorithm allows for optimization of computational costs based on desired precision, available computational resources, system temperatures, densities, and size. We are delivering the theory, initial applications, and software required to motivate and facilitate the widespread adoption of our new algorithm. This will constitute a significant leap in nations ability to model the microscopic physics of matter at extreme conditions.

Publications

Journal Articles

Malko, S., W. Cayzac, V. Ospina-Bohorquez, K. Bhutwala, M. Bailly-Grandvaux, C. McGuffey, R. Fedosejevs, X. Vaisseau, A. Tauschwitz, J. Apinaniz, D. De Luis, G. Gatti, M. Huault, J. Perez-Hermandez, S. Hu, A. J. White, L. A. Collins, P. Neumayer, G. Faussurier, J. Vorberger, G. Prestopino, C. Verona, J. Santos, D. Batani, F. N. Beg and L. Volpe. Proton stopping measurements at low velocity in warm dense carbon. Submitted to *Nature Communications*. (LA-UR-21-28294)

Sharma, V., L. A. Collins and A. J. White. Stochastic and Mixed Density Functional Theory within the projector augmented wave formalism for the simulation of warm dense matter. Submitted to *Physical Review Letters*. (LA-UR-23-20795)

*White, A. J., L. A. Collins, K. Nichols and S. X. Hu. Mixed stochastic-deterministic time-dependent density functional theory: application to stopping power of warm dense carbon. 2022. *Journal of Physics: Condensed Matter*. **34** (17): 174001. (LA-UR-21-31679 DOI: 10.1088/1361-648X/ac4f1a)

Reports

White, A. J. IC Annual Report 1st year: w21_udft. Unpublished report. (LA-UR-22-22871)

Presentation Slides

Nichols, K. A., A. J. White, L. A. Collins and S. Hu. Investigating the Stopping Power of Warm Dense Plasmas using Time-Dependent Mixed Density-Functional Theory (TD-mDFT). Presented at *APS DPP*, Pittsburgh, Pennsylvania, United States, 2021-11-09 - 2021-11-09. (LA-UR-21-30711)

Nichols, K. A., A. J. White, S. X. Hu, V. N. Goncharov, L. A. Collins and D. Mihaylov. Investigation of Nonlocal Electron Transport in High-Energy-Density Plasmas using Ab Initio Methods. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30669)

Sharma, V., A. J. White and L. A. Collins. Mixed Stochastic-Deterministic Density Functional Theory Within The PAW Formalism: An Efficient Approach to Warm Dense Matter. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30767)

White, A. J. Ab Initio Dynamics of Matter in Extreme Conditions: Hybrid Stochastic-Deterministic Density Functional Theory. Presented at *PNNL Theory and Plasma Science and Technology Seminar*, Virtual, New Mexico, United States, 2022-05-31 - 2022-05-31. (LA-UR-22-24956)

White, A. J. New ab initio methods for electron and Ion transport properties of matter extreme conditions: from electronic stopping power to ion diffusion.. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30894)

White, A. J. SHRED: An open-source DFT code for exascale and matter in extreme conditions. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-05 - 2023-03-10. (LA-UR-23-22307)

White, A. J. IC Project w21_udft from Solids to Plasmas: A Universal Approach to Ab Initio Modeling Across Temperature Regimes. . (LA-UR-23-23284)

White, A. J., L. A. Collins, K. A. Nichols and S. Hu. Time-Dependent Mixed Deterministic-Stochastic Kohn Sham Density Functional Theory for Matter in Extreme Conditions. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21867)

Posters

White, A. J. Nonequilibrium Dynamics of Materials in Extreme Conditions : Ab initio simulation of stopping of high energy projectiles by warm dense matter. . (LA-UR-21-29192)

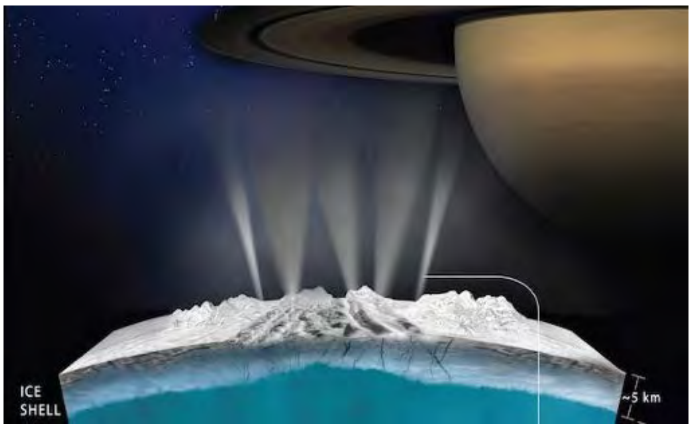
Other

White, A. J. Ab Initio Dynamics of Matter in Extreme Conditions: Hybrid Stochastic-Deterministic Density Functional Theory. Audio/Visual. (LA-UR-22-26403)

**Peer-reviewed*

Multiscale Method for Fluid-Kinetic Coupling in Ocean-World Jet Simulations

Daniel Livescu
20210298ER



Artist's rendition of Enceladus hydrothermal activity. Credit: NASA. The project aims to perform the first kinetic / fluid coupled simulations of the jets using our new approach, and provide scaling formulas to relate the far field observations to the flow properties at the surface vent.

Project Description

Many problems of importance to Department of Energy (DOE)/National Nuclear Security Administration (NNSA) cover regimes where atomistic effects are important, but at scales where kinetic calculations are not possible. Examples extend from flows at microscales in Inertial Confinement Fusion, to stockpile applications, to earth's magnetic field and space weather, and to astrophysics. There is an urgent need for accurate calculations of such applications, and this is currently a very active area of research with a plethora of multiscale approaches, which also underlines the difficulty of the problem. Our multiscale method relies on a very promising approach, ensuring premier high-fidelity, but computationally efficient calculations. The application we have chosen to demonstrate the approach is timely in light of the National Aeronautics and Space Administration's (NASA's) planned space missions, but lacks any pertinent calculation to date. Thus, our first ever calculations of Enceladus/Europa water jets will guide future space missions by helping understand jet source conditions and also estimating forces/stresses on probes/landers expected to be dropped in those jets. In addition, the cost-efficient multiscale method developed in this work could facilitate spatially multi-dimensional simulations coupling hydrodynamic phenomena with dense plasma and kinetic effects encountered in DOE/NNSA specific applications.

Publications

Journal Articles

Corbetta, A., A. Gabbana, V. Gyrya, D. Livescu, J. Prins and F. Toschi. Towards learning Lattice Boltzmann collision operators. Submitted to *European Physical Journal E. Soft Matter*. (LA-UR-22-33173)

Sharan, N. and J. Bellan. Investigation of high-pressure turbulent jets using direct numerical simulation. Submitted to *Journal of Fluid Mechanics*. (LA-UR-21-26442)

*Wei, T., D. Livescu and X. Liu. Scaling patch analysis of planar turbulent wakes. 2022. *Physics of Fluids*. **34** (6): 065116. (LA-UR-22-24624 DOI: 10.1063/5.0097588)

Wei, T., X. Liu, Z. Li and D. Livescu. Effects of pressure gradients on planar turbulent wakes. Submitted to *Physical Review Fluids*. (LA-UR-22-32624)

Wei, T., Z. Li and D. Livescu. Scaling patch analysis of planar turbulent mixing layers. 2022. *Physics of Fluids*. **34** (11): 115120. (LA-UR-22-29141 DOI: 10.1063/5.0122494)

Wei, T. and D. Livescu. Scaling of the mean transverse flow and Reynolds shear stress in turbulent plane jet. Submitted to *Physics of Fluids*. (LA-UR-21-20834)

Wei, T. and D. Livescu. Scaling analysis of turbulent planar plume. Submitted to *Physics of Fluids*. (LA-UR-21-23862)

Presentation Slides

Brady, P. T. and D. Livescu. High-Order Cut-Cell Methods for High-Fidelity Flow Simulations. Presented at *International Conference on Computational Fluid Dynamics*, Maui, Hawaii, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26667)

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Objective discovery of fluid dynamical regimes with unsupervised machine learning. Presented at *American Physical Society Division of Fluid Dynamics Fall Meeting*, Phoenix, Arizona, United States, 2021-11-22 - 2021-11-22. (LA-UR-21-31365)

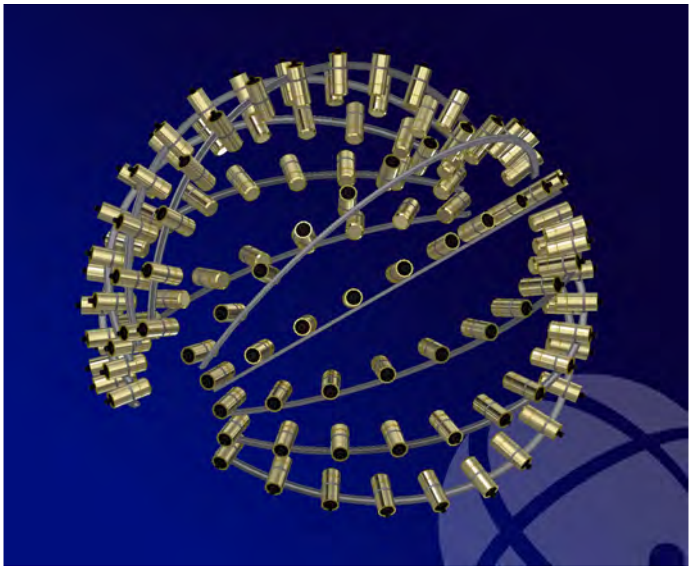
Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Objective discovery of dominant dynamical regimes. Presented at *Machine Learning for Climate (Kavli Institute for Theoretical Physics)*, Santa Barbara, California, United States, 2021-11-01 - 2021-11-04. (LA-UR-21-31428)

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Objective discovery of dominant dynamical regimes. Presented at *Machine Learning for Climate (Kavli Institute for Theoretical Physics)*, Santa Barbara, California, United States, 2021-11-01 - 2021-11-04. (LA-UR-21-31437)

**Peer-reviewed*

Towards Actinide Scattering Measurements at the Los Alamos Neutron Science Center

Keegan Kelly
20210329ER



Shown here is a preliminary design for the proposed detector. Each detector is a novel, newly available CLYC-6 detector (neutron-gamma detector) capable of near perfect neutron-gamma separation, orders of magnitude of neutron energy measurements, and excellent signal timing. This array will allow for next generation measurements of neutron scattering at LANL.

Project Description

Neutron scattering is the most common neutron reaction on fissionable and non-fissionable nuclei, and thus information on these poorly-known reactions is essential for descriptions of fission-driven systems. We aim to provide unparalleled measurements of these reactions with highly-restrictive cross-reaction correlations to provide a breakthrough in the accuracy with which Department of Energy/National Nuclear Security Administration mission-relevant systems can be studied. Additionally, the never-before-measured correlations between these reactions and other neutron-induced reactions will severely limit the extent to which nuclear data libraries can be varied to match criticality benchmarks, thereby potentially revealing other lingering and previously unknown nuclear data errors in other reactions of interest.

Publications

Journal Articles

Kelly, K. J., J. M. O'Donnell, J. A. Gomez, M. Devlin and E. A. Bennett. The impact of detection rate changes and correlations on random-coincidence background measurements. 2023. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **1045**: 167531. (LA-UR-22-26334 DOI: 10.1016/j.nima.2022.167531)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Correlated n-\xce\xb3 Angular Distributions from the 12C(n,n#1) Reaction for Incident Neutron Energies from 6.5–16.5 MeV. Submitted to *Physical Review C*. (LA-UR-21-21204)

Conference Papers

Kelly, K. J., E. A. Bennett, M. J. Devlin, J. M. O'Donnell and M. W. Paris. The Neutron Scattering Cross Section and Angular Distribution Measurement Program at LANL. Presented at *International Conference on Nuclear Data for Science and Technology*. (Los Alamos, New Mexico, United States, 2022-07-22 - 2022-07-29). (LA-UR-22-30435)

Presentation Slides

Bennett, E. A. Direct Measurements of Neutron Scattering at LANSCE. Presented at *Low Energy Community Meeting*, Los Alamos, New Mexico, United States, 2021-08-09 - 2021-08-11. (LA-UR-21-28103)

Bennett, E. A. Design and Simulation of a Next-Generation Dual n-gamma Detector Array at Los Alamos National Laboratory. Presented at *Division of Nuclear Physics Conference 2021*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-14. (LA-UR-21-30190)

Bennett, E. A., K. J. Kelly, M. J. Devlin and J. M. O'Donnell. Design and Commissioning of a Next-Generation Dual n-gamma Detector Array at Los Alamos National Laboratory. Presented at *International Conference on Nuclear Data for Science and Technology*, Livermore, California, United States, 2022-07-25 - 2022-07-29. (LA-UR-22-27478)

Couture, A. J. Fast Neutron Physics at LANSCE. Presented at *Neutrons for Science (NFS) Workshop 2022*, Caen, France, France, 2022-04-13 - 2022-04-13. (LA-UR-22-23317)

Kelly, K. J. Development in Neutron Scattering at WNR using Dual n-gamma Detection. . (LA-UR-21-23850)

Kelly, K. J. Neutron Scattering and Future Experimental Capabilities at WNR. Presented at *LANSCE Futures Spring Workshop 2021: Nuclear Science*, LOS ALAMOS, New Mexico, United States, 2021-05-10 - 2021-05-11. (LA-UR-21-24514)

Kelly, K. J. LANL ``What Do We Get'' Report. . (LA-UR-22-20570)

Kelly, K. J., E. A. Bennett, M. J. Devlin and J. M. O'Donnell. Towards Actinide Scattering Measurements at LANSCE Project 20210329ER 2022 LDRD Appraisal. . (LA-UR-22-32464)

Kelly, K. J., M. A. Mosby and T. Kawano. Dual n-gamma Measurement of the 235U(n,3n) Cross Section. . (LA-UR-21-29859)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell, E. A. Bennett and M. W. Paris. LANL Updates on Chi-Nu and Neutron Scattering. Presented at *CSEWG 2021*, Upton, New York, United States, 2021-11-15 - 2021-11-19. (LA-UR-21-31496)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell, E. A. Bennett and M. W. Paris. The Neutron Scattering Cross Section and Angular Distribution Measurement Program at LANL. Presented at *15th International Conference on Nuclear Data for Science and Technology (ND2022)*, Los Alamos, New Mexico, United States, 2022-07-22 - 2022-07-28. (LA-UR-22-27552)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell, M. W. Paris and E. A. Bennett. White Source n-gamma Coincidence Measurements of gamma-Production Cross Sections at LANSCE. . (LA-UR-21-30669)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. LANSCE Experimental Updates II: Neutron Scattering at WNR. Presented at *2020 Cross Section Evaluation Working Group*, Upton, New York, United States, 2020-11-30 - 2020-12-04. (LA-UR-20-29952)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Development of Dual n-gamma Techniques at the Los Alamos Neutron Science Center. Presented at *SORMAWest 2021*, N/A, New Mexico, United States, 2021-05-14 - 2021-05-21. (LA-UR-21-24477)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Prompt Fission Neutron Detection and Neutron Scattering Measurements at WNR FP15L. . (LA-UR-21-30485)

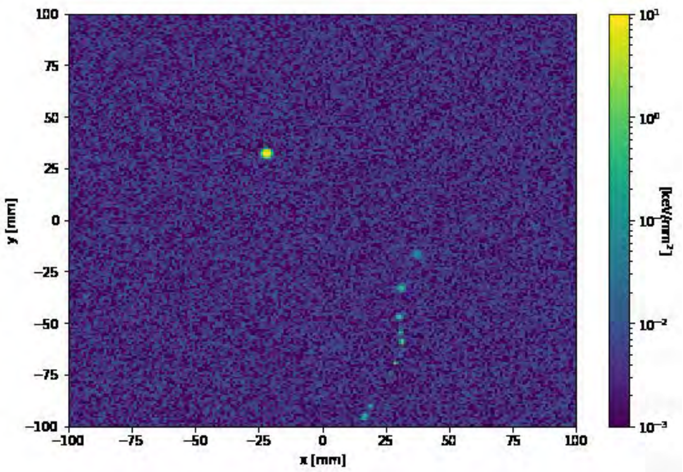
Posters

Bennett, E. A., K. J. Kelly, M. J. Devlin and J. M. O'Donnell. Design and Simulation of a Next-Generation Dual n-gamma Detector Array at LANL. Presented at *IEEE Symposium on Radiation Measurements and Applications (SORMA West)*, Berkeley, California, United States, 2021-05-19 - 2021-05-28. (LA-UR-21-24796)

**Peer-reviewed*

Unmasking Dark Matter with the Migdal Effect

Steven Elliott
20210499ER



A simulated event from our studies to optimize the shielding. The event shows an electron-positron pair tracks at the lower right and a nuclear recoil in the upper left.

Project Description

This effort will develop a directionally sensitive measurement for neutrons. The driving goal of the experiment is the full understanding of existing and proposed dark matter experiments, a major set of investments by Department of Energy (DOE). While it is conceivable that the technology could be used for neutron detection, the underlying purpose is the measurement of a key atomic-nuclear physics effect that is the foundation of many dark matter searches.

Publications

Presentation Slides

Colgan, J. P. Unmasking Dark Matter with the migdal effect. . (LA-UR-22-21509)

Massarczyk, R. Chasing neutrinos a mile underground. . (LA-UR-20-29252)

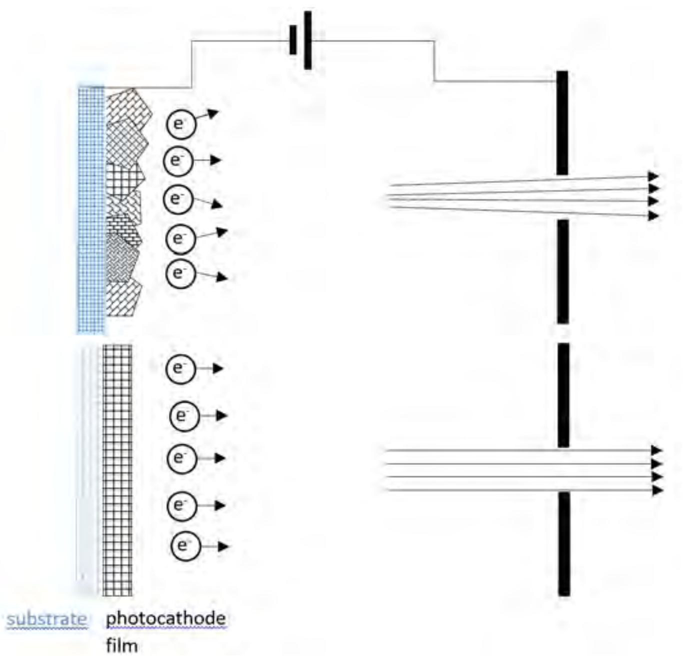
Posters

Colgan, J. P. and M. S. Pindzola. Neutron-impact ionization of the carbon atom. Presented at *DAMOP 2021*, Online, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25164)

**Peer-reviewed*

Molecular Beam Epitaxy of Alkali Antimonide Photocathodes

Vitaly Pavlenko
20220058ER



Although in accelerators electrons eventually reach relativistic speeds, even a tiniest amount of their velocities (energy) in transverse directions at the origin (cathode) matters. Mean transverse energy (MTE) of the photoemitted electrons defines how tightly they can be kept focused along the beamline. Disorder in a polycrystalline film structure (top) leads to larger MTE. If a single crystalline film can be grown on top of a lattice-matched substrate (bottom), MTE can be drastically reduced. This study will pursue alkali antimonide epitaxial growth in the Applied Cathode Enhancement and Robustness Technology (ACERT) laboratory, relying on a recently developed stoichiometry control method.

Project Description

Future hard X-ray free electron lasers – billion-dollar-class facilities - are considered essential for sustainable stockpile stewardship. Their reliable operation and performance depend on a tiny but critical piece, a photocathode (laser-triggered source of electrons). Moreover, future hard X-ray sources will either require photocathodes that are beyond today's state-of-the-art or would be able to significantly extend their design parameters if/when such electron sources are available. Namely, single crystalline photocathodes with high quantum efficiency are required. Materials that can be prepared in single crystalline form today such as metals have fundamentally low quantum efficiency. High quantum efficiency materials such as alkali antimonides so far can only be produced as polycrystalline films. Relying on the automated growth technology that we recently innovated, we are working on developing a method that will produce single crystalline thin films for a complicated case of alkali antimonide compounds.

Publications

Journal Articles

*Pavlenko, V., J. Smedley, A. Scheinker, R. L. Fleming, A. Alexander, M. A. Hoffbauer and N. A. Moody. Stoichiometry control and automated growth of alkali antimonide photocathode films by molecular beam deposition. 2022. *Applied Physics Letters*. **120** (9): 91901. (LA-UR-21-30432 DOI: 10.1063/5.0080948)

Presentation Slides

Freibert, F. J. Clementine Reactor and Pu Aging: Irradiation Induced Modifications in \xce\xb4-PuGa Alloys. . (LA-UR-22-22488)

Pavlenko, V. Automated growth of photocathode films: from the basics of process control towards artificial intelligence. Presented at *Photocathode Physics for Photoinjectors (P3) Workshop*, Menlo Park, California, United States, 2021-11-10 - 2021-11-12. (LA-UR-21-31176)

Pavlenko, V. Automated Growth of Photocathodes. . (LA-UR-22-20586)

Pavlenko, V. Alkali antimonide cathodes for photoinjectors: Toward reliable fabrication methods. Presented at *LCLS-II-HE Collaboration: Technical Seminar Series*, Menlo Park, California, United States, 2022-04-15 - 2022-04-15. (LA-UR-22-23388)

Pavlenko, V. Automated Growth of Photocathodes. Presented at *DisrupTECH*, Los Alamos, New Mexico, United States, 2022-08-03 - 2022-08-03. (LA-UR-22-27760)

Pavlenko, V. Stoichiometry control and automated growth of alkali antimonide photocathode films by molecular beam deposition. Presented at *European Workshop on Photocathodes for Particle Accelerator Applications (EWPAA 2022)*, Milano, Italy, 2022-09-20 - 2022-09-22. (LA-UR-22-29768)

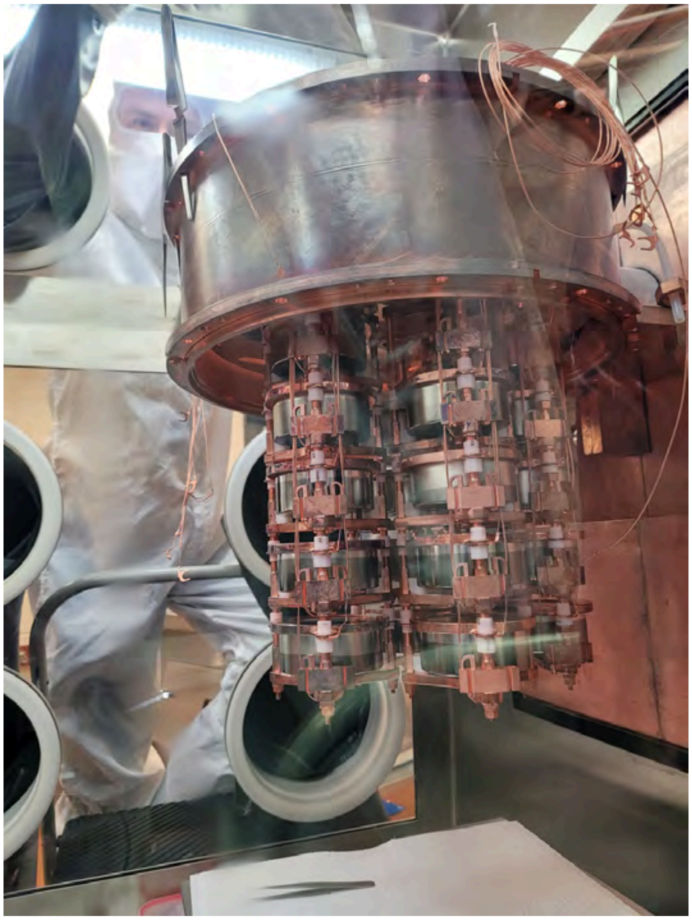
Posters

Pavlenko, V. Alkali Antimonide Photocathode Thin Film Growth: from Sequential Deposition Towards Automated Process Control.. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-28193)

**Peer-reviewed*

The Decay of Nature’s Rarest Isotope

Ralph Massarczyk
20220092ER



Co-Pi Sam Meijer working on the opened cryostat of the MAJORANA germanium detector array in March 2021. During his stay in the clean room of the underground facility, he rewired the signal connection of the individual detector units. The tantalum disks will be installed in between the germanium crystal inside the clean copper structure.

Project Description

To search for nature's rarest nuclear decay we must use dedicated techniques in radiation detection and data analysis in ultra-clean environments. We plan to find one of the last missing radioactive decays which has never been observed, but plays a role in our understanding in nuclear and astrophysics. We are leveraging the opportunity that became available when a Department of Energy-funded experiment ended its data taking period, and building on its experience to illustrate how to search for ultra-rare decay signatures. At the same time we want to search for the expected rare signatures of dark matter, and transfer the knowledge and talent to Los Alamos National Laboratory's mission relevant efforts, like the search for rare signature in nuclear forensics.

Publications

Presentation Slides

Massarczyk, R. Current Status of MJD, MJD-Ta, and LEGEND. Presented at *SURF User Association General User Meeting*, online, New Mexico, United States, 2022-10-26 - 2022-10-27. (LA-UR-22-31285)

Massarczyk, R. and S. Schleich. The decay of natures rarest isotope. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Nuclear Physics (DNP)*, New Orlans, Louisiana, United States, 2022-10-27 - 2022-10-31. (LA-UR-22-31283)

Posters

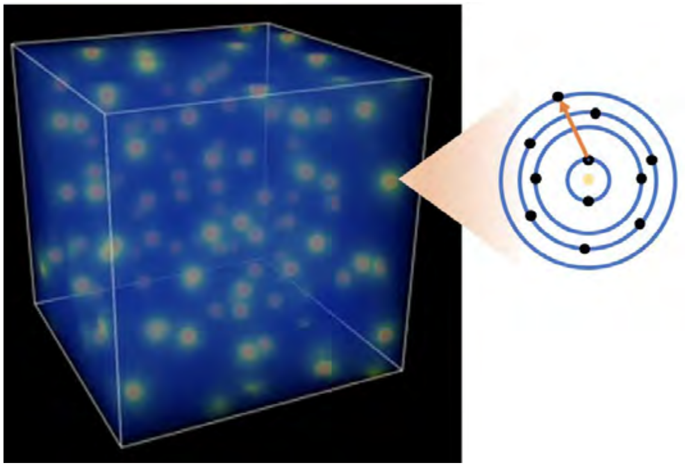
Massarczyk, R., S. J. Meijer, P. Chu and S. R. Elliott. The Decay of Nature's Rarest Isotope. Presented at *Majorana Public Webinar for final announcements*, Lead, South Dakota, United States, 2023-02-23 - 2023-02-23. (LA-UR-23-21726)

Massarczyk, R. and S. Schleich. Using ultra-clean conditions of the Majorana Demonstrator to measure unobserved 180mTa decay. Presented at *SDSMT Undergrad Poster Symposium*, Rapid City, South Dakota, United States, 2022-04-05 - 2022-04-05. (LA-UR-22-23375)

**Peer-reviewed*

Excited States in Warm Dense Matter

Charles Starrett
20220172ER



Accurate modeling of the electronic structure of warm dense matter requires the explicit simulation of many atoms (left picture) to capture the plasma physics effects, together with a detailed structure calculation for the many excited states (right picture) to capture the atomic physics. The purpose of this project is to accurately combine these effects into a single model.

Project Description

Accurate knowledge of the material properties of warm dense matter is key to our ability to model phenomena such as fusion energy and core Los Alamos National Laboratory mission needs. Our proposal combines the best techniques from two separate but fundamentally related fields (equation of state and atomic physics), into a single consistent and accurate method. The resulting code will provide state-of-the-art understanding and benchmark calculations, and address open and enigmatic experimental measurements. This transformative approach will allow us to rule out, or in, the role of consistent plasma physics in key experimental measurements of energy transport with light, that currently disagree with our best models.

Publications

Journal Articles

Starrett, C. E. and N. R. Shaffer. Average Atom Model with Siegert States. Submitted to *Physical Review E*. (LA-UR-22-32687)

Presentation Slides

Diaz, L. I. and S. A. Alber. Understanding Warm Dense Matter beyond Density Functional Theory. Presented at *XCP summer workshop*, Los Alamos, New Mexico, United States, 2022-08-18 - 2022-08-18. (LA-UR-22-28811)

Starrett, C. E. Multi-Center Calculations of the Opacity at Very High Pressure. . (LA-UR-22-21945)

Starrett, C. E. Average-Atom-Type Models for Warm Dense Matter. Presented at *Multiscale Modeling of Matter under Extreme Conditions*, Gorlitz, Germany, 2022-09-12 - 2022-09-12. (LA-UR-22-29234)

Posters

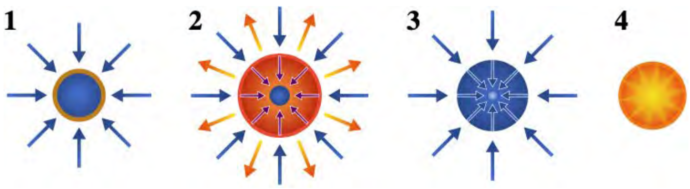
Diaz, L. I. and S. A. Alber. Understanding Warm Dense Matter beyond Density Functional Theory. . (LA-UR-22-28327)

Starrett, C. E. and N. R. Shaffer. An Exact Treatment of the Free Electron Continuum with Discrete States. Presented at *Radiative Properties of Hot Dense Matter*, Santa Fe, New Mexico, United States, 2022-11-14 - 2022-11-14. (LA-UR-22-31330)

**Peer-reviewed*

Kinetic Electron and Radiation Transport in Inertial Confinement Fusion (ICF)-capsule Implosions

Luis Chacon
20220200ER



An ICF-capsule evolution comprises four main stages: (1) radiation impinges upon the capsule surface, turning its outer layer into hot plasma; (2) the central thermonuclear fuel is compressed and heated by the rocket force of the expanding plasma layer; (3) the fuel reaches up to 20x lead density and few hundred million K; (4) the fuel ignites and burns (Image credit: http://en.wikipedia.org/wiki/File:Inertial_confinement_fusion.svg). Modern ICF-design codes neglect many important physical mechanisms, thereby significantly over-predicting the capsule performance. Fully-kinetic, bleeding-edge LANL code iFP incorporates lots of missing physics and is used to assess its importance.

Project Description

Achieving ignition-grade plasmas in the laboratory is critical for stockpile stewardship. In fact, the inertial-confinement-fusion (ICF) Ignition and High Yield Program is one of four major Science, Technology, and Engineering elements of the nuclear-weapons Stockpile Stewardship Program, the main responsibility of the Department of Energy/National Nuclear Security Administration. Contrary to numerical-simulations predictions, the National Ignition Facility (NIF) has failed to ignite, demonstrating wide gaps in our simulation capabilities and theoretical understanding of ICF-capsule implosions. Recently, we have completed development of the next-generation ICF-simulation capability that accounts for a multitude of physics effects, which are neglected by the standard ICF-simulations tools. Here, we will use this capability to study and quantify importance of several such effects.

Publications

Presentation Slides

Chacon, L. Modern multiscale kinetic algorithms for high-fidelity ICF capsule and hohlraum simulations. . (LA-UR-23-21005)

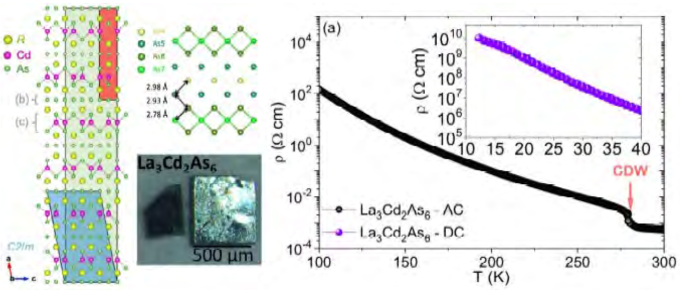
Chacon, L., S. E. Anderson, G. Chen, A. J. Stanier and W. T. Taitano. Formulation and Solvers for Kinetic-Fluid Models for Plasma Simulation. Presented at *SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP22)*, Virtual, Washington, United States, 2022-02-23 - 2022-02-23. (LA-UR-22-21381)

Hammer, H. R., L. Chacon, S. E. Anderson and A. N. Simakov. Beyond radiation-hydrodynamics Coupling kinetic plasma and radiation transport. Presented at *17th Copper Mountain Conference On Iterative Methods*, Virtual, New Mexico, United States, 2022-04-04 - 2022-04-08. (LA-UR-22-23065)

**Peer-reviewed*

Narrow-Gap Semiconductors for Sub-Mega Electron Volt (MeV) Dark Matter Detection

Sean Thomas
20220252ER



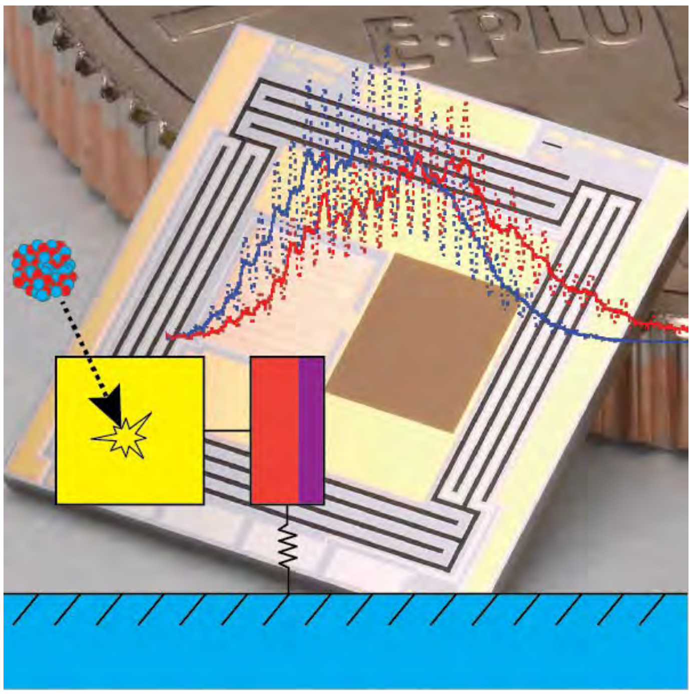
La3Cd2As6 is a newly discovered narrow-gap semiconductor that shows promise as a dark matter, infrared, and high-resolution x-ray detector. We will explore it suitability for these purposes with an emphasis on the ultimate goal of dark matter detection. Here, we show its crystal structure, a photo of a single crystal, and its resistivity, demonstrating its narrow gap behavior. Adapted from Piva et al., Chem. Mat., 33, 4122 (2021).

Project Description

Innovation in detector technologies for dark matter searches with novel materials and advanced techniques to new regimes of sensitivity are Los Alamos National Laboratory and Department of Energy priorities. It has recently been predicted that a sufficiently clean narrow-gap semiconductor could serve as the basis for a dark matter detector in the low-mass regime. Such a material was recently discovered at Los Alamos, and this project will evaluate its suitability for dark matter detection. This is a unique window of opportunity for Los Alamos to develop new dark matter experimental capabilities and position itself as a leader in this field.

Fission Fragment Spectroscopy Beyond the 1 Atomic Mass Unit (AMU)

Matthew Carpenter
20220282ER



Transition-edge sensor detectors can achieve new levels of performance in radiation detection. In this image, a schematic of a fission fragment being absorbed and detected in the gold absorber of a sensor operating below 100 millikelvins is superimposed on top of a picture of a LANL transition-edge sensor chip along with simulated fission fragment spectra of uranium-235 and californium-252 measured with our sensors.

Project Description

Understanding the process of nuclear fission is important to nuclear energy, nuclear security, and other areas like nuclear forensics of nuclear material release from events like Fukushima. This project will develop and test a new type of radiation detector that may dramatically improve current experiments to measure fission fragments at Los Alamos, allowing us to probe fission reactions and their products in greater detail. To do accomplish this, we will adapt a detector technology called the Transition Edge Sensor (TES) to be able to measure the energy ranges of fission fragments, and study the technical challenges required to deploy this type of detector to a fission fragment experiment at the Los Alamos Neutron Science Center (LANSCE). The expected outcome is a validated sensor design and specification, along with engineering specifications for the cryogenic instrumentation needed to build a fission fragment spectrometer for LANSCE.

Publications

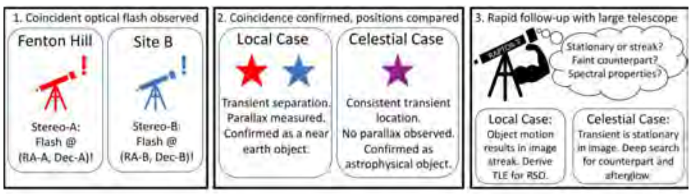
Presentation Slides

Carpenter, M. H., M. P. Croce, D. G. McNeel, K. A. Schreiber, J. N. Ullom, D. A. Bennett, J. A. B. Mates, J. D. Gard, J. Imrek, D. T. Becker, A. L. Wessels and K. M. Morgan. Ultra-High-Resolution Cryogenic X-Ray Spectrometer for Advanced Electron Microscope Actinide Material Mapping. Presented at *Applied Superconductivity Conference 2022*, Honolulu, Hawaii, United States, 2022-10-23 - 2022-10-28. (LA-UR-22-31171)

**Peer-reviewed*

What is the Origin of Sub-Second Optical Flashes in the Night Sky?

W Vestrand
20220288ER



Stereoscopic imaging of optical flashes is the key to discriminating sub-second satellite glints from astrophysical flashes on an event-by-event basis. This cartoon shows how we independently identify flash candidates at two robotic telescope sites and compare the apparent flash locations to derive the parallax of the flash. The 38 kilometer separation of the telescopes allows parallax ranging of glints out to a distance of ten times the distance of the Moon. Coincident sub-second flashes without a measurable parallax are astrophysical candidates. Both types of flashes will be identified in real time and followed-up with observations by more powerful interrogating telescopes.

Project Description

Wide-area searches for sub-second optical flashes from the Night Sky have recently become practical because of advances in affordable, high frame rate, optical sensors and commercial off-the-shelf (COTS) wide-field telescopes. The first results from those surveys indicate the existence of previously unknown sub-second optical flashes in the night sky. Most flashes are probably fast glints from a population of high altitude satellites and poorly characterized orbital debris. Understanding the nature of that glinting orbital debris is essential for space protection and enabling better space traffic management for Department of Energy/National Nuclear Security Administration space missions. So we will conduct the first comprehensive study of that potentially lethal debris. Many models of explosive behavior in extreme astrophysical environments also predict the generation of sub-second optical flashes, so there is considerable also excitement in the astronomical community over the possibility that some of the flashes could have an astrophysical origin. Our stereoscopic, wide-field, telescope array will be the first capable of discriminating sub-second satellite glints from astrophysical flashes in real time on an event-by-event basis. We will therefore also use the system to search for astrophysical transients and, if identified, use our more powerful, narrow field, robotic telescopes to explore the physics of those extreme astrophysical explosions.

Publications

Journal Articles

Panaitescu, A. D. and W. T. Vestrand. The Synchrotron Low-energy Spectrum Arising from the Cooling of Electrons in Gamma-Ray Bursts. 2022. *The Astrophysical Journal*. **938** (2): 132. (LA-UR-22-25196 DOI: 10.3847/1538-4357/ac8b75)

Panaitescu, A. D. and W. T. Vestrand. Properties of the Prompt Optical Counterpart Arising from the Cooling of Electrons in Gamma-Ray Bursts. 2022. *The Astrophysical Journal*. **938** (2): 155. (LA-UR-22-28294 DOI: 10.3847/1538-4357/ac9315)

Conference Papers

Vestrand, W. T., Y. H. Sechrest, L. P. Parker, R. J. J. Hill, D. Palmer and P. R. Wozniak. Exploring the Nature of Sub-Second Optical Flashes in the Night Sky. Presented at *SPIE Astronomical Telescopes and Instrumentation*. (Montreal, Canada, 2022-07-19 - 2022-07-23). (LA-UR-22-26941)

Vestrand, W. T., Y. H. Sechrest, R. J. J. Hill, D. Palmer, L. P. Parker, M. W. Vance and P. R. Wozniak. Exploring a new class of bright, ultra-fast, glints from resident space objects. Presented at *Advanced Maui Optical and Space Surveillance Technologies Conference (AMOS)*. (Kahului, Hawaii, United States, 2022-09-27 - 2022-09-30). (LA-UR-22-29109)

Presentation Slides

Vestrand, W. T. Exploring a new class of bright, ultra-fast, glints from resident space objects. Presented at *Advanced Maui Optical and Space Surveillance Technologies Conference (AMOS)*, Kahului, Hawaii, United States, 2022-09-27 - 2022-09-30. (LA-UR-22-29523)

Vestrand, W. T., Y. H. Sechrest, L. P. Parker, R. J. J. Hill, D. Palmer and P. R. Wozniak. Exploring the Nature of Sub-Second Optical Flashes in the Night Sky. Presented at *SPIE Astronomical Telescopes and Instrumentation 2022*, Montreal, Canada, 2022-07-19 - 2022-07-23. (LA-UR-22-26966)

Vestrand, W. T., Y. H. Sechrest, R. J. J. Hill, M. J. Giblin, D. Palmer, L. P. Parker and P. R. Wozniak. Stereoscopic Ranging of Sub-Second Optical Flashes in the Night Sky. Presented at *38th New Mexico Symposium*, Socorro, New Mexico, United States, 2023-02-17 - 2023-02-17. (LA-UR-23-21661)

Vestrand, W. T., Y. H. Sechrest, R. J. J. Hill, M. J. Giblin, D. Palmer, L. P. Parker and P. R. Wozniak. Stereoscopic Ranging of Sub-Second Optical Flashes in the Night Sky. Presented at *AGN: Santa Fe*, Santa Fe, New Mexico, United States, 2023-03-22 - 2023-03-24. (LA-UR-23-22772)

Posters

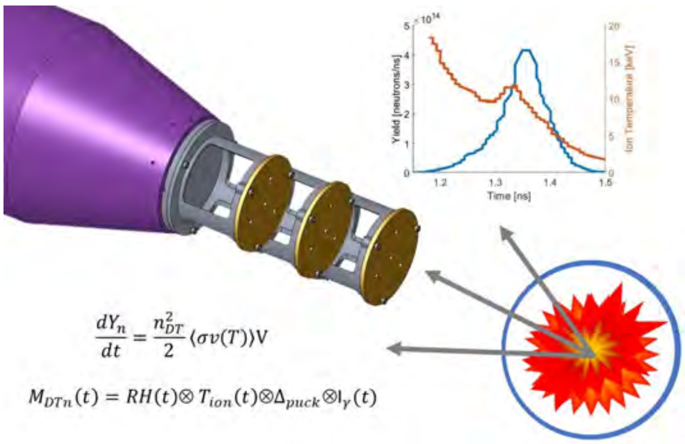
Vestrand, W. T., Y. H. Sechrest, R. J. J. Hill, D. Palmer, L. P. Parker, M. W. Vance and P. R. Wozniak. Exploring a new class of bright, ultra-fast, glints from resident space objects. Presented at *Advanced Maui Optical and Space Surveillance Technologies Conference (AMOS)*, Kahului, Hawaii, United States, 2022-09-27 - 2022-09-30. (LA-UR-22-29292)

**Peer-reviewed*

Time Resolved Temperature of Burning Plasmas with Multi-Puck Array

Kevin Meaney

20220294ER



How the temperature evolves in a burning inertial confinement fusion capsule is one of the most sensitive metrics of capsule performance and energy balance of the fusion hot spot. A multi-puck array measuring the specific broadening of the fusions neutrons escaping can allow us to measure how this temperature evolves and give deep insight into burning plasmas.

Project Description

Inertial confinement fusion experiments support the stockpile by creating ultra extreme environments. One of the most sensitive factors is the ion temperature - how hot the plasma becomes and how the temperature evolves throughout the implosion. Right now, the ion temperature averaged over the fusion burn is measured, but not how the temperature changes with time. This project will develop a diagnostic technique that will measure particles being emitted from the nuclear fusion process and use them to measure the time resolved ion temperature. The time resolved ion temperature will be used to gain a deeper understanding about inertial confinement fusion implosions and be used to collect data about how various effects affect the ion temperature. This dataset will be fed into physics simulation codes to test their ability to accurately predict this novel observation. Furthermore, the diagnostic system will be able to continue to collect data across implosions across high energy density facilities around the nation.

Publications

Journal Articles

*Meaney, K. D., Y. Kim, N. M. Hoffman, H. Geppert-Kleinrath, J. Jorgenson, M. Hochanadel, B. Appelbe, A. Crilly, R. Basu, E. Y. Saw, A. Moore and D. Schlossberg. Design of multi neutron-to-gamma converter array for measuring time resolved ion temperature of inertial confinement fusion implosions. 2022. *Review of Scientific Instruments*. **93** (8): 083520. (LA-UR-22-25428 DOI: 10.1063/5.0101887)

Presentation Slides

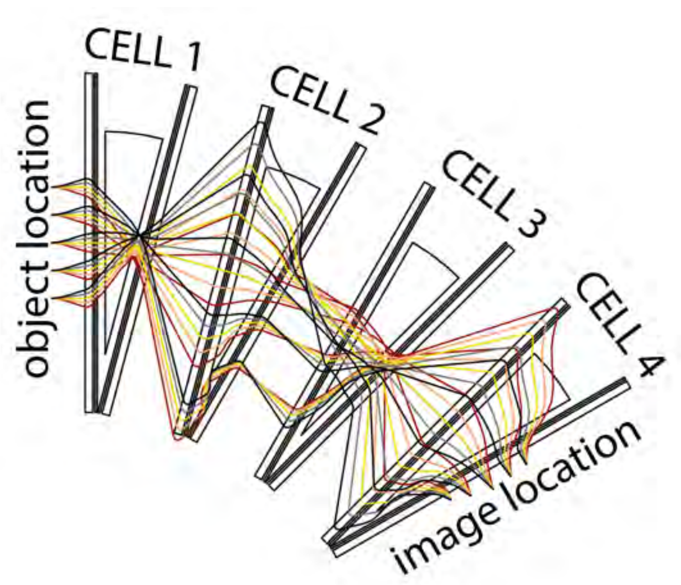
Meaney, K. D. 2023 Shot Request - MultiPuck + HTTemp. . (LA-UR-22-22672)

Meaney, K. D. 2024 Shot Request - MultiPuck + HT Mix Time. . (LA-UR-23-20743)

**Peer-reviewed*

High Depth-of-Field Proton Radiography

Fesseha Mariam
20220343ER



The achromat imaging system visualized here in concept will focus the proton distribution, through a dense object of widely varying density, onto an imaging plane distal from the object. This will enable the visualization of objects much larger and density than previously possible, opening up new possibilities for the types of mid-scale experiments that can probed by pRad, and closing in on the gap in the capabilities of the National Nuclear Security Administration complex that now exist between proton radiography (pRad) and the Dual Axis Radiographic Hydrodynamic Test (DARHT) facility.

Project Description

800-Mega electron-volt (MeV) proton radiography, as implemented at the Los Alamos Neutron Science Center (LANSCE) facility (proton radiography (pRad)), regularly interrogates dense materials on rapid timescales. The thickness through which an object can be visualized, however, is limited by the chromatic (i.e., blurring) effects of the lensing system. This work seeks to overcome that blur, by introducing additional lensing elements, to make the lens achromatic. This will have the effect of removing the contributions of blur to the system intrinsic to thicker systems with a broad range of densities to be probed. The end result will be a scaling up of the type of experiment that can be performed at the pRad facility, to enable much thicker experiments, opening up new possibilities for the studies of equations of state, and the vetting of more complex hydrodynamic modeling relevant to future weapons needs.

Publications

Reports

Schanz, M., J. C. Allison, F. G. Mariam, M. S. Freeman, L. P. Neukirch and J. L. I. Schmidt. IAC Beam Characterization V2.0. Unpublished report. (LA-UR-22-32173)

Schanz, M., J. C. Allison, M. S. Freeman, F. G. Mariam and L. P. Neukirch. IAC Beam Characterization Measurements. Unpublished report. (LA-UR-22-27250)

Presentation Slides

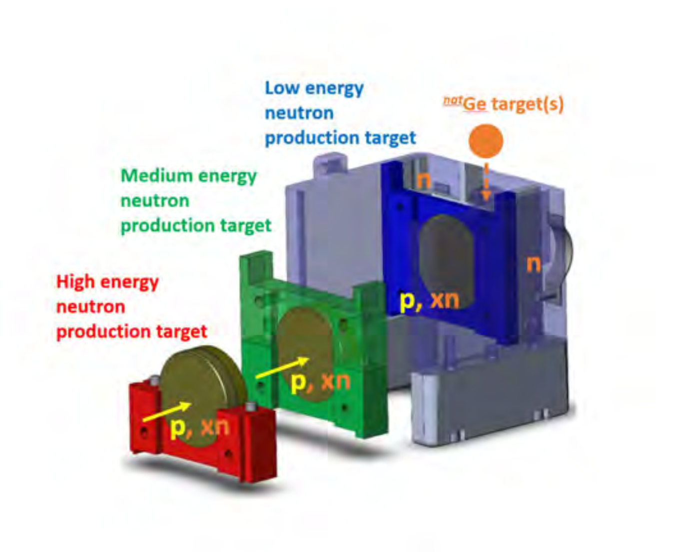
Mariam, F. G., J. C. Allison, M. S. Freeman, L. P. Neukirch, M. Schanz, J. L. I. Schmidt and E. Valetov. Achromatic Imaging Using Charged Particles. Presented at *43rd International Workshop on High-Energy-Density Physics*, Hirschegg, Austria, 2023-01-29 - 2023-02-03. (LA-UR-23-20797)

Schanz, M. Development of Achromatic Imaging Capabilities for pRad at LANSCE. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-28021)

**Peer-reviewed*

Creating a Germanium-68 Source for Neutrinoless Double Beta-Decay Detectors

Ellen O'Brien
20220722ER



This is a schematic of the Isotope Production Facility (IPF) production stack with high, medium, and low energy neutron production targets upstream of the neutron-slot (n-slot) target irradiation location. The n-slot target irradiation location will be used to generate Ge-68 from natural Ge targets and to characterize the secondary neutron flux energy spectrum and spatial distribution. germanium-68 (Ge-68) will be embedded in a high purity germanium detector to probe the backgrounds seen in neutrinoless double beta decay. Characterization of the secondary neutron spectrum will allow for investigation of radioisotopes that can be produced in this location in the IPF target stack.

Project Description

"We propose to irradiate a high purity natural germanium sample using the secondary neutron flux at the Los Alamos National Laboratory Isotope Production Facility (IPF) to produce a small quantity of the radioisotope germanium-68 and to thoroughly characterize the secondary neutron flux at this facility. If successful, the irradiated sample can be used to create a germanium detector with a uniformly embedded germanium-68 source. The detector to be created with this sample is outside the scope of this proposal. The successful production of germanium-68 and its uniform infusion into a germanium detector will be of significant value in the quantification of the background present in the search for neutrinoless double beta decay, and will provide a unique capability that has not been realized elsewhere. This is in support of the Laboratory's mission to be at the forefront of discovery in nuclear and particle physics. In addition, the further development and characterization of the secondary neutron spectrum at Los Alamos' Isotope Production Facility will inform the feasibility of new, "alternative" production pathways, and may enhance its ability to produce mission critical isotopes for the Department of Energy (DOE) Isotope Program."

Publications

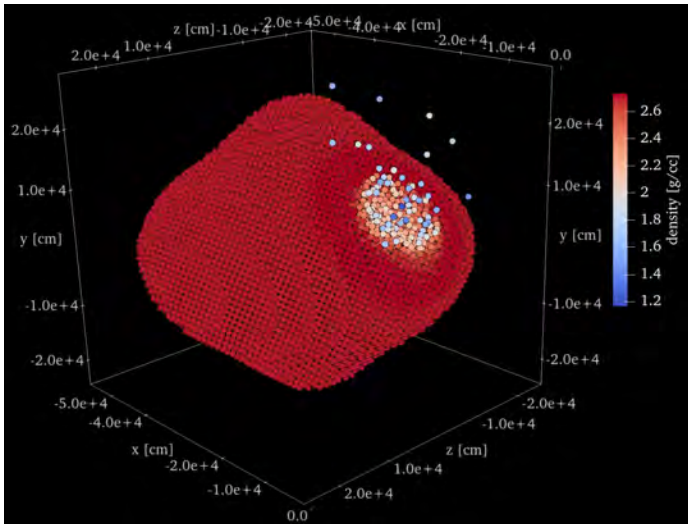
Reports

O'Brien, E. M. and J. T. Morrell. Summary of N-Slot Irradiation at IPF. Unpublished report. (LA-UR-22-31754)

**Peer-reviewed*

Can Asteroids be Pulverize-It?

Irina Sagert
20220771ER



An example of how the team will simulate Pulverize-It scenarios using smoothed particle hydrodynamics code FleCSPH. Shown is a top-shaped basalt asteroid that was set up via FleCSPH. The asteroid was hit by a projectile, represented by a single smooth particle hydrodynamics (SPH) particle at 10kilometers per second. The image shows the crater formation and material ejection. The team used about 50,000 SPH particles. In full simulations of realistic Penetrator-Interceptor (PI) scenarios, the team will use orders of magnitude more particles to increase resolution as well as a field of PI penetrators instead of a single object.

Project Description

The project will evaluate the effectiveness of the Penetrator-Interceptor (PI) method for planetary defense. This recently proposed method is a rapid response option to mitigate asteroid and comet impacts on Earth. Due to its novelty, the PI method has not been tested by numerical studies which can use state-of-the-art models for asteroid materials and include an object's spin and shape. This project will be the first one to use such numerical methods for fluid and solid dynamics to provide an understanding of outcomes of the PI approach in realistic impact scenarios. The proposed work focuses on modeling high-velocity impacts of man-made projectiles into asteroids and comets and directly contributes to the National Nuclear Security Administration (NNSA)-National Aeronautics and Space Administration (NASA) planetary defense partnership. The team will use the Hayabusa2 and Double Asteroid Redirection Test (DART) missions to benchmark the numerical method, and will tie the studies to international and NASA space missions. The planned development and application of numerical methods will result in a complex multi-physics code that scales to the largest machines available and can be applied to high-velocity impact scenarios which cannot be achieved in the laboratory. This will benefit the Advanced Scientific Computing program by contributing to Verification and Validation as well as Physics and Engineering efforts.

Publications

Reports

Tong, L. N., O. Korobkin and I. Sagert. Kuiper Belt Fender Benders: morphogenesis of contact-binary KBOs using FleCSPH. Unpublished report. (LA-UR-22-24904)

Presentation Slides

Sagert, I., C. M. Mauney, G. D'Angelo and A. J. Josephson. Towards Creating a Numerical Pipeline for Climate Effects of Asteroid Impacts. Presented at *Asteroid Impacts Global Effects*, Virtual, New Mexico, United States, 2022-07-13 - 2022-07-13. (LA-UR-22-26487)

Tong, L. N. Formation of Bi-Lobed Kuiper Belt Objects through the Kozai-Lidov Mechanism. . (LA-UR-22-24911)

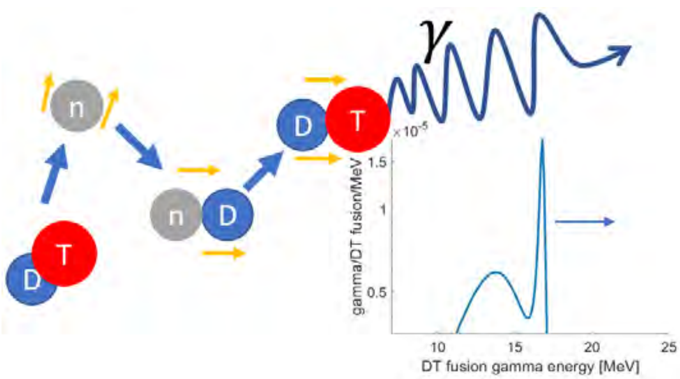
Tong, L. N. Chaos and Periodicity in Quadrupole-Monopole Binaries. . (LA-UR-22-28392)

Tong, L. N. Scale-Free Dynamics of Monopole-Quadrupole Binaries Applied to the Morphogenesis of Bi-lobed KBOs. Presented at *American Physical Society (APS) 4 Corners Meeting*, Albuquerque, New Mexico, United States, 2022-10-14 - 2022-10-15. (LA-UR-22-30870)

**Peer-reviewed*

Measuring Reaction-in-Flight Fusion Reactions Through High-Energy Gamma Rays

Kevin Meaney
20220785ER



In inertial confinement fusion, up-scattered reactions from the fusion process give information about the mix and stopping power of the dense, burning plasma - valuable diagnostic information. Often measured with radiochemistry techniques, such reaction-in-flight measurements are often under-constrained. In this project, the team investigates an alternative, complementary pathway to measure reaction-in-flight interactions through ultra-high energy gamma rays to potentially open a novel pathway and nuclear interaction to measure this valuable interaction.

Project Description

Inertial confinement fusion (ICF) experiments undergo rare nuclear interactions that up-scatter neutron energies higher than what nuclear fusion normally creates. By measuring these higher-than-expected neutrons, we can infer the amount of shell mix into the nuclear fusion hot spot - an extremely important metric of performance. In ICF experiments on the National Ignition Facility (NIF), so few of these neutrons are made, it is difficult to constrain the models that relate them to mix. This project will develop theoretical nuclear physics calculations to measure these up-scattered processes through a gamma ray path instead of the neutron path. Calculating the expected super high energy gamma rays will allow us to understand what needs to be done to measure this effect through an alternative technique. If successful, we can either make a first of its kind measurement on the NIF or define the diagnostic requirements needed to do so. Making a clean measurement will help diagnose, understand and improve ICF performance.

Publications

Journal Articles

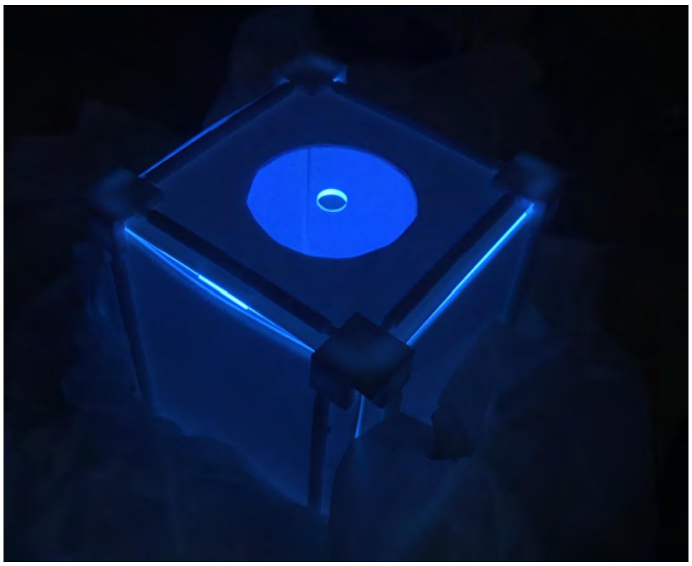
Meaney, K. D., M. W. Paris, G. M. Hale, Y. H. Kim and A. C. Hayes-Sterbenz. Deuterium-Tritium Fusion Gamma Ray Spectrum at MeV Energies with Application to Reaction-in-Flight Inertial Confinement Fusion Measurements. Submitted to *Physical Review C*. (LA-UR-23-23201)

**Peer-reviewed*

Ultra-Cold Neutron Experiment for Proton Branching Ratio in Neutron Beta Decay (UCNProBe)

Zhaowen Tang

20190048ER



The prototype central detector array for UCNProBe project under ultraviolet light, the blue light is generated by scintillators which form the walls of the detector. The team plans to contain the ultracold neutrons inside this scintillator box and simultaneously detect the electrons from neutron beta decays. The result of this study has the potential to help resolve the neutron lifetime anomaly.

Project Description

The free neutron decay lifetime is vital across many fields of physics. The Department of Energy Office of Science, Nuclear Physics has identified resolving the beam and bottle neutron lifetime discrepancy as a prerequisite to the next generation neutron lifetime experiments. The successful execution of this project will position the Laboratory to solve this lifetime discrepancy. The confirmation of the bottle lifetime results will be a vital piece of information for the nuclear physics community and help pave the way for a next generation ultracold neutron (UCN) based lifetime experiment; the confirmation of the beam lifetime results would demonstrate beyond the Standard Model (SM) of physics, and be truly extraordinary.

Technical Outcomes

The team has successfully executed a number of research and development tasks for a new neutron lifetime experiment. The team was able to assemble and test a prototype detector design that will guide the improvements of the final experiment.

Publications

Journal Articles

*Tang, Z., E. B. Watkins, S. M. Clayton, S. A. Currie, D. E. Fellers, M. T. Hassan, D. E. Hooks, T. M. Ito, S. K. Lawrence, S. W. T. MacDonald, M. Makela, C. L. Morris, L. P. Neukirch, A. Saunders, C. M. O'Shaughnessy, C. Cude-Woods, J. H. Choi, A. R. Young, B. A. Zeck, F. Gonzalez, C. Y. Liu, N. C. Floyd, K. P. Hickerson, A. T. Holley, B. A. Johnson, J. C. Lambert and R. W. Pattie. Ultracold neutron properties of the Eljen-299-02D deuterated scintillator. 2021. *Review of Scientific Instruments*. **92** (2): 023305. (LA-UR-20-27508 DOI: 10.1063/5.0030972)

Presentation Slides

Hassan, M. T. An experiment to measure the Proton Branching Ratio in Neutron Beta Decay (UCNProBe). Presented at *APS DNP 2019*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30666)

Hassan, M. T. The current status of the UCNProBe experiment. Presented at *APS DNP 2021*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-30177)

Morris, C., Z. Tang and N. C. Floyd. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *LUG 2022*, Los Alamos, New Mexico, United States, 2022-06-02 - 2022-06-03. (LA-UR-22-26659)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *Particle Physics with Neutrons at the ESS*, stockholm, Sweden, 2018-12-10 - 2018-12-14. (LA-UR-18-31486)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *APS April Meeting 2019*, denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23299)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *Fundamental physics with neutron beta decay*, Seattle, Washington, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31233)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *CIPANP 2022*, Lake Buena Vista, Florida, United States, 2022-08-30 - 2022-09-04. (LA-UR-22-29128)

Tang, Z. The Los Alamos ultracold neutron source. Presented at *LANSCE 50th Anniversity*, Los Alamos, New Mexico, United States, 2022-09-07 - 2022-09-09. (LA-UR-22-29281)

Tang, Z., C. Morris, J. H. Choi and D. E. Fellers. Search for the Neutron Decay n\xe2\x9f\xb6\xf0\x9d\x9b\xbe+X, where X is a dark matter particle. Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30026)

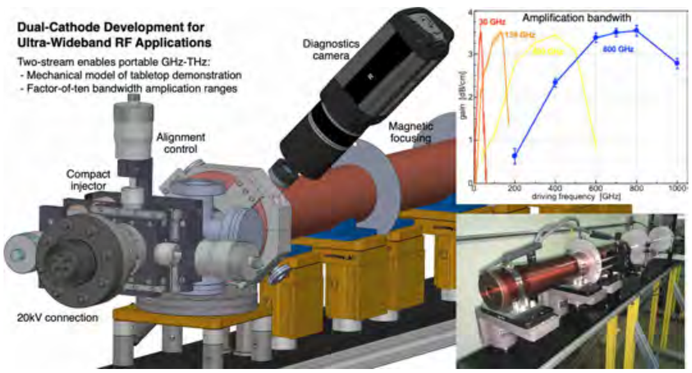
Tang, Z., J. C. Lambert, C. Morris and S. Clayton. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30027)

Tang, Z. and N. C. Floyd. Ultra-Cold Neutron measurement of the Proton branching ratio in neutron Beta Decay (UCNProBe). Presented at *APS DNP 2020*, Virtual, New Mexico, United States, 2020-10-29 - 2020-11-02. (LA-UR-20-28876)

**Peer-reviewed*

Wideband Sub-Millimeter Source for Deployed Applications

Kip Bishofberger
20190066ER



Ultra-high bandwidth, including gigahertz (GHz) and terahertz (THz) ranges, is an extremely useful capability for portable active interrogation and communications applications. The dual-cathode demonstration is shown at left, and the amplifier performance is shown in upper right. Each range shows the capability at a specific set of voltages. Ranges are dialed in only by adjusting voltage range.

Project Description

We are developing a wideband amplifier system that can yield significant power over a wide range of frequencies. The system is compact and power-efficient for low size, weight, and power applications. Project results could potentially impact several Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) mission areas. Several potential future applications are described below. Project results could impact Mono/bistatic Radar Time-domain Spectroscopy. Results from this project could ultimately support a capability to probe a cloud, smoke column, or atmospheric region. A large bandwidth would allow one system to be used to detect a wide variety of chemical signatures. Project results could impact Space-based Spectroscopy; future applications could allow most of the atmospheric column to be analyzed via a system deployed from orbit. Project results could impact Secure Communications; a small wavelength would enable small antennas to communicate (at very high bandwidths), without unintended listeners (e.g., satellites, aircraft, binoculars). Project results could impact Materials Inspection; although dielectrics are transparent, the high resolution anticipated through this project would ultimately allow the detection of millimeter-scale features (e.g., high-Z, circuitry) for improvised explosive device (IED) and special nuclear material (SNM detection).

Technical Outcomes

The project successfully evaluated the performance of the electron injector (electron gun) in support of the two-stream instability project. The experimental team was able to have a dual-cathode injector developed and built that was used to confirm that beam parameters match those in the original objectives.

Publications

Journal Articles

*Yampolsky, N. and K. Bishofberger. Description of longitudinal space charge effects in beams and plasma through dielectric permittivity. 2021. *Physics of Plasmas*. **28** (8): 083103. (LA-UR-21-21464 DOI: 10.1063/5.0057436)

Conference Papers

Neben, D. E., K. A. Bishofberger, V. Pavlenko and N. Yampolsky. Design of a Source for Millimeter-wave Ultra-wide Bandwidth Applications Using the Two-stream Instability. Presented at *International Vacuum Electronics Conference*. (Monterey, California, United States, 2020-04-20 - 2020-04-23). (LA-UR-20-21994)

Presentation Slides

Neben, D. E. Ultra Wide Bandwidth Source Utilizing the Two Stream Instability. . (LA-UR-21-27587)

Posters

Neben, D. E., N. Yampolsky, K. A. Bishofberger and V. Pavlenko. Design of a Source for Millimeter-wave Ultra-wide Bandwidth Applications Using the Two-Stream Instability. Presented at *IVEC 2020*, Monterey, California, United States, 2020-10-17 - 2020-10-17. (LA-UR-20-27600)

Neben, D. E., N. Yampolsky, V. Pavlenko and K. A. Bishofberger. A TEST SOURCE FOR THE PRODUCTION OF MILLIMETER-WAVE RF USING THE TWO-STREAM INSTABILITY. Presented at *ICOPS 2020*, Los Alamos, New Mexico, United States, 2020-12-06 - 2020-12-06. (LA-UR-20-29912)

**Peer-reviewed*

Ultralight Bosonic Dark Matter Search with an Optically Pumped Magnetometer

Leanne Duffy
20190113ER

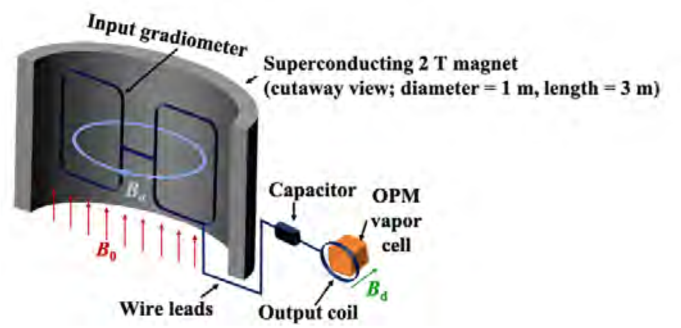


Illustration of the axion dark matter detection scheme using an inductor-capacitor (LC) circuit with an optically pumped magnetometer (OPM). The presence of dark matter axions in the strong magnetic field (B0) induces a tiny magnetic field (Ba). The capacitor is used to tune the resonant frequency of the circuit to try to amplify and detect this effect at the output using the OPM.

Project Description

Modern cosmological observations lead to the conclusion that most of the matter in the Universe is of an undiscovered form. Matter that interacts with light contributes only 20% of the Universe's matter, with the remaining 80% given by dark matter, inferred via its gravitational effects on visible matter and radiation. Discovering the nature of dark matter is one priority of Cosmic Frontier research funded by the Department of Energy Office of Science, High Energy Physics program. Los Alamos National Laboratory has a unique intersection of leadership in axion physics with world-leading magnetic field detection capabilities through the development and application of optically pumped magnetometers, and an existing magnet that can be applied to develop the next level of sensitivity in axion searches. We estimate that our proposed experiment can probe axion specific axion masses with a sensitivity that is up to 4 orders of magnitude beyond the existing best limit. Our ultimate goal is to reveal the nature of the Universe's dark matter. At the very least, we will provide significant new limits on the properties of the dark matter.

Technical Outcomes

This project is the first use of an Optically Pumped Magnetometer (OPM) as the sensitive magnetometer in searching for ultralight dark matter. The team designed, optimized, and built a detection circuit suitable for a prototype axion dark matter search. The team also successfully acquired background data with the experiment, and demonstrated reduction of the background noise with the cooling of the magnet shield.

Publications

Reports

Milton, S. V. Review of LDRD ER Project 20190113ER. Unpublished report. (LA-UR-21-20385)

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Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)

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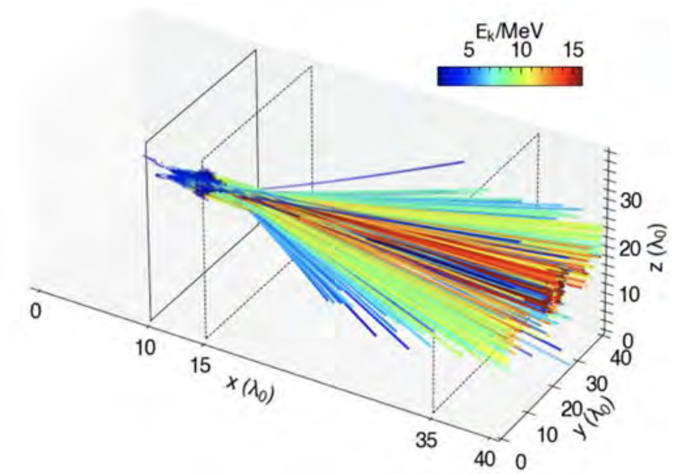
**Peer-reviewed*

Hot Electron Beam Generation and Transport for Fast Ignition

Sasikumar Palaniyappan
20190124ER



Three-dimensional particle-in-cell (PIC) simulation shows how electrons undergo vaccum-laser-acceleration (VLA) when an intense laser interacts with a thin foil. Electrons gain substantial energy away from the original foil location when they get injected into the laser beam and accelerated further by the VLA process. This is the first demonstration of VLA in a transmission geometry which is crucial for generating a good electron beam using a laser.

Project Description

Inertial confinement fusion (ICF) is one of the grand challenges of this century due to its potential to provide an unlimited amount of clean energy. In laser-driven ICF, a high-energy nanosecond laser compresses a mixture of deuterium (D) and tritium (T) fuel inside a capsule to very high-density and temperature and initiates nuclear fusion reactions. Despite decades of research, laboratory fusion is still elusive. Electron fast ignition is a variant of ICF where the fuel is first compressed to high density using a long-pulse (nanosecond) laser and then ignited by a hot-electron beam generated from a short-pulse (picosecond) laser interaction with a gold cone tip, where the short pulse laser is usually brought into the assembled dense fuel via a re-entrant cone. The current cone-in-shell design suffers due to large electron beam divergence. This proposal will address the crippling deficiencies in electron fast ignition by generating a near-collimated hot-electron beam using near-critical plasmas and transport it effectively from the source to the dense fuel with the aid of resistive magnetic collimation.

Technical Outcomes

The primary objective of the project was to mitigate the detrimental effects of laser pre-pulse inside the gold re entrant cone and generate the hot electron beam from the gold cone tip rather than from the gold cone side wall. The project successfully demonstrated laser pre-pulse mitigation using a plasma absorber in an experiment at OMEGA Laser Facility. This will have large impact in electron fast ignition, and in laser-driven x-rays, protons, and neutron sources.

Publications

Journal Articles

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Li, F., P. K. Singh, S. Palaniyappan and C. Huang. Parameterization of nonlinear particle resonances in direct laser acceleration. Submitted to *Physical Review Letters*. (LA-UR-20-22447)

Singh, P. K., F. Li, C. Huang, A. Moreau, R. Hollinger, S. A. Junghans, A. Favalli, C. Calvi, S. Wang, Y. Wang, H. Song, J. Rocca, R. E. Reinovsky and S. Palaniyappan. Multi-stage MeV electron acceleration from laser-driven nano-foils undergoing relativistic transparency. Submitted to *Nature Physics*. (LA-UR-21-20711)

Singh, P. K., F. Li, S. A. Junghans, A. Favalli, R. E. Reinovsky, C. Huang, S. Palaniyappan, A. Moreau, R. Hollinger, C. Calvi, S. Wang, Y. Wang and J. J. Rocca. Cascade acceleration of MeV electrons during intense femtosecond laser-nanometer foil transparency. Submitted to *Physical Review Letters*. (LA-UR-20-24689)

Reports

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Presentation Slides

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Li, F. Laser-plasma based electron acceleration and its applications. . (LA-UR-20-24276)

Li, F., C. Huang, P. K. Singh and S. Palaniyappan. Electron beam properties from combined direct laser acceleration and plasma acceleration in regimes relevant to fast ignition. Presented at *49th Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-14. (LA-UR-19-25253)

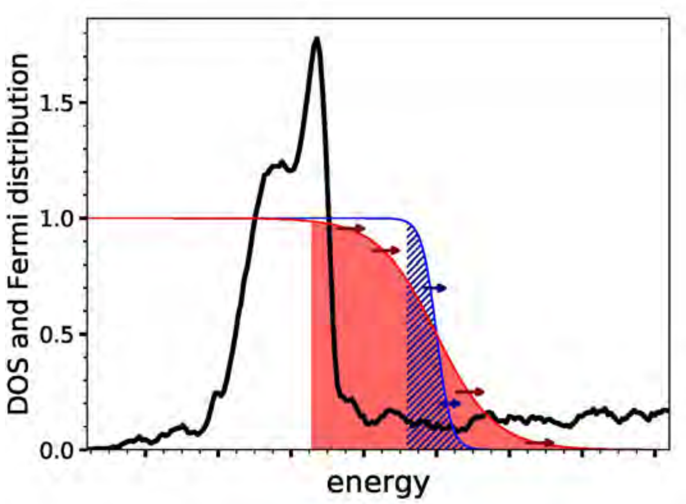
Li, F., C. Huang, P. K. Singh and S. Palaniyappan. Towards controlled laser acceleration of electrons in laser-plasma coupling regimes relevant to fast ignition. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30695)

Singh, P. K., F. Li, S. A. Junghans, C. Huang, A. Favalli, R. E. Reinovsky, S. Palaniyappan, A. Moreau, R. Hollinger, C. Calvi, S. Wang, Y. Wang, H. Song and J. J. Rocca. Cascade acceleration of MeV electrons during intense femtosecond laser-nanometer foil transparency. Presented at *62nd Annual Virtual Meeting of the APS Division of Plasma Physics.*, Los Alamos, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29242)

**Peer-reviewed*

Effects of Strong Electronic Correlations on the Properties of Warm Dense Matter

Jerome Daligault
20200074ER



In order to understand the physical properties of a material in the warm dense matter regime, we are developing theoretical tools to study and predict how the interactions of its constituent electrons between themselves and with their environment vary with temperature. The figure illustrates the distribution of energy levels (black line) of electrons in warm dense copper and their probability of being occupied for two different temperatures, 2000 Kelvin (blue line) and 20000 Kelvin (red); the colored area indicate those electrons that play a central role in determining, e.g., the electric and thermal conductivity of the material.

Project Description

The issues we address affect national energy and security missions at Los Alamos, which require high-fidelity computer simulations that rely on accurate plasma properties over a wide range of physical conditions, and in particular of warm dense matter (WDM) conditions that occur during the implosion phase of inertial confinement fusion capsules. By its intermediate nature, the WDM regime does not fall neatly within the parameter space typical of either ordinary condensed-matter physics or plasma physics, and the standard simplifying approximations of these fields no longer apply. As a consequence, our theoretical understanding of this extreme state of matter relies mostly on advanced computer simulations. The new computational tool we will develop in this project will significantly advance our predicting capability of properties of WDM. This will be a new, world-class capability to model extreme states of matter at the Laboratory that will support both discovery research and programmatic applications at the forefront of an exciting and rapidly growing field. We will apply our much-improved electronic structure calculations to several pressing questions in support of current and future experiments.

Technical Outcomes

The project developed advanced theoretical and numerical tools for understanding and modeling warm dense matter. The primary results of this project include: (i) a unique simulation tool that allows first-principle determination of electronic correlations under warm dense matter (WDM) conditions; (ii) first kinetic theory of electrons and ions in WDM and its implications; (iii) a thorough study of finite-temperature effects on electronic correlations in a reference model; (iv) a collaboration to an ongoing WDM experiment.

Publications

Journal Articles

*Bernstein, D. J., T. Lafleur, J. Daligault and S. D. Baalrud. Friction force in strongly magnetized plasmas. 2020. *Physical Review E*. **102** (4): 041201. (LA-UR-20-23660 DOI: 10.1103/PhysRevE.102.041201)

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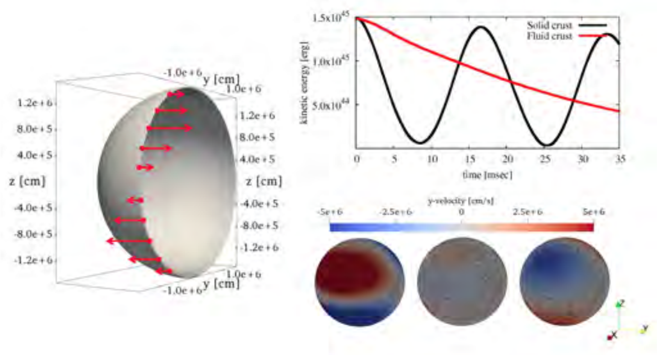
**Peer-reviewed*

Exploration of Neutron-Star Crust Dynamics in the Era of Gravitational-Wave Astrophysics

Irina Sagert

20200145ER



A shell representing parts of the neutron star crust in a smoothed particle hydrodynamics simulation tool, FleCSPH. Red arrows indicate shear velocities to simulate the fundamental toroidal oscillation mode of the crust as observed after giant X-ray flares. When described as a solid, the crust undergoes oscillations, seen in the kinetic energy evolution. When no material strength is included, the kinetic energy decays due to numerical viscosity. The resulting oscillation frequency is ca. 25 hertz which is close to observations. This test shows that solid material modeling in FleCSPH can describe the dynamics of the crust, an important step towards exploring crust dynamics in binary mergers.

Project Description

This project will quantify of the role of the solid neutron-star crust in neutron-star mergers. Dynamical studies of mergers with realistic microphysical input have only recently become feasible. We will be the first ones to include the solid crust. Neutron-star material is too dense and neutron-rich to be attained in laboratories and its study complements experiments as done by e.g. the Facility for Rare Isotope Beams. In our work, we will disentangle its effect from the nuclear equation of state in gravitational wave and electromagnetic signatures of merger events. Our results will be crucial for gravitational wave detectors like the Laser Interferometer Gravitational-wave Observatory (LIGO) and Virgo, and be important for gamma-ray observatories as the National Aeronautics Space Administration's Fermi and Chandra missions. This work will use state-of-the-art nuclear physics input to answer fundamental questions about the states of matter following the Department of Energy's Long Range Plan of Nuclear Science. We will deliver complex multi-physics codes that scale to the largest machines available and apply these codes in the to the most extreme conditions that exist in the universe. This will benefit the Advanced Scientific Computing Program by providing insights into improving simulation capability, reliability, and scalability.

Technical Outcomes

The project delivered a multi-physics code, FleCSPH, which is able to model the dynamics of fluids and solids in terrestrial and astrophysical setups. The team modeled the 3-dimensional dynamics of the solid neutron-star crust in shear oscillations for the very first time which can be compared to observational data that is extracted from giant X-ray flares. At the end of the project, the team began the first simulations of neutron-star binaries with a solid crust.

Publications

Journal Articles

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*W. R. T. *. F. C. L. *. H. A. L. *. R. S. *. F. C. J. *. M. M. R. *. C. E. A. *. E. W. P. *. M. J. *. M. G. W. *. L. J. Korobkin, O. *., O. Korobkin, R. T. Wollaeger, C. L. Fryer, A. L. Hungerford, C. J. Fontes, M. R. Mumpower, E. A. Chase, W. P. Even, G. W. Misch, J. Lippuner and J. Miller. Axisymmetric Radiative Transfer Models of Kilonovae. 2021. *The Astrophysical Journal*. **910** (2): 116. (LA-UR-20-22607 DOI: 10.3847/1538-4357/abe1b5)

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Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *Spheric 2021*. (Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11). (LA-UR-21-24191)

Reports

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Korobkin, O. Institutional Computing 2019/2020 Allocation Report: Viewgraphs, Year 1. Unpublished report. (LA-UR-20-25615)

Lim, H. FleCSPH Wiki. Unpublished report. (LA-UR-20-26581)

Tong, L. N., O. Korobkin and I. Sagert. Kuiper Belt Fender Benders: morphogenesis of contact-binary KBOs using FleCSPH. Unpublished report. (LA-UR-22-24904)

Presentation Slides

Korobkin, O. Mergers of Compact Objects with SPH and General Relativity, Allocation: w20_nsmergers (year 1). . (LA-UR-21-22056)

Korobkin, O. Simulations of Compact Object Binary Mergers with FleCSPH: Allocation Report (t22_compactm). . (LA-UR-23-23387)

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Lim, H. Are we alone? Searching Intelligent Life Beyond the Earth. . (LA-UR-20-25542)

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Sagert, I., O. Korobkin, B. Tsao and H. Lim. Studying Crust-Breaking Events in Neutron Stars with Strength and Smoothed Particle Hydrodynamics. . (LA-UR-21-21876)

Sagert, I., O. Korobkin, M. A. R. Kaltenborn, H. Lim, J. Loiseau, C. M. Mauney, I. Tews, B. Tsao and W. P. Even. Overview of FleCSPH Solid Material Modeling Capabilities. . (LA-UR-21-25175)

Sagert, I. and O. Korobkin. Studying Crust-Breaking Events in Neutron Stars with Strength and Smoothed Particle Hydrodynamics. . (LA-UR-20-21887)

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Tong, L. N. Scale-Free Dynamics of Monopole-Quadrupole Binaries Applied to the Morphogenesis of Bi-lobed KBOs. Presented at *American Physical Society (APS) 4 Corners Meeting*, Albuquerque, New Mexico, United States, 2022-10-14 - 2022-10-15. (LA-UR-22-30870)

Tsao, B. Smooth Particle Hydrodynamics for Neutron Star Oscillation with General Relativistic effects. Presented at *LANL Astrophysics seminar*, Los Alamos, New Mexico, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-22758)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *SPHERIC 2021*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25313)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *SPHERIC 2021*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25319)

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Korobkin, O. Fully Dynamical General Relativistic SPH: Progress and Challenges. Presented at *The 25th Anniversary Four Corners Meeting of the American Physical Society*, Albuquerque, New Mexico, United States, 2022-09-14 - 2022-10-15. (LA-UR-22-30235)

Lim, H., O. Korobkin, J. Loiseau, C. M. Mauney, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *American Physical Society (APS) April Meeting 2022*, Virtually Anywhere, New Mexico, United States, 2022-04-09 - 2022-04-12. (LA-UR-22-22754)

Lim, H., O. Korobkin, J. M. Miller, R. T. Wollaeger, C. J. Fontes, M. A. R. Kaltenborn, W. P. Even and J. Loiseau. Studying Expansion of Ejecta from Binary Neutron Star Mergers. Presented at *Aps April Meeting 2021*, Virtually Anywhere, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23238)

Tsao, B., O. Korobkin, H. Lim, I. Sagert, I. Tews and J. Loiseau. Studying Neutron Star Oscillations with General Relativistic Smoothed Particle Hydrodynamics. Presented at *APS April meeting 2021*, virtual, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23327)

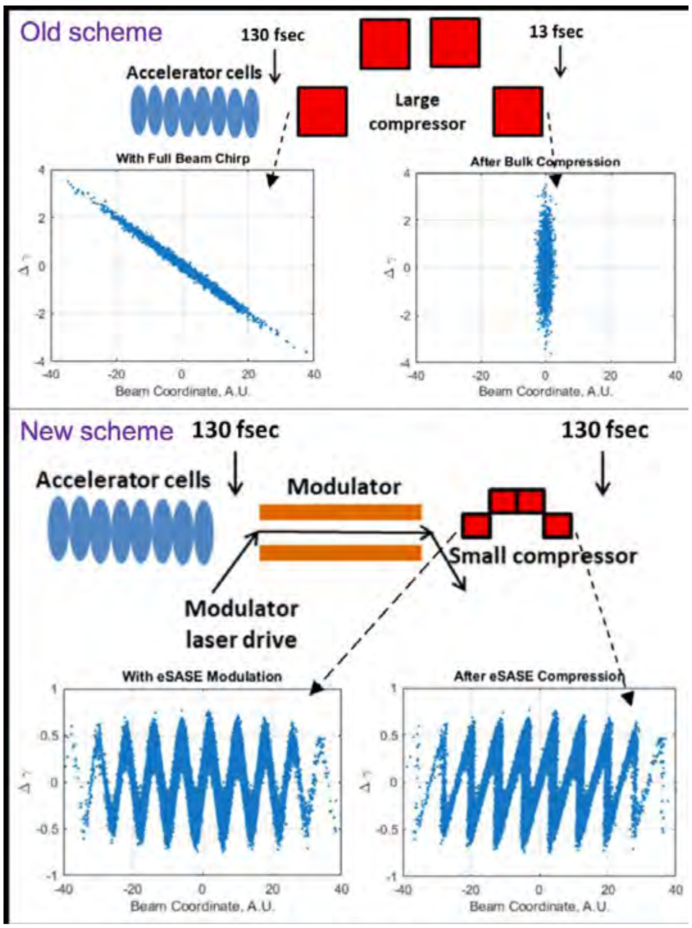
Other

Lim, H. Are we alone? Searching Intelligent life beyond the Earth. Audio/Visual. (LA-UR-20-27695)

**Peer-reviewed*

Novel X-ray Free-Electron Lasers (XFEL) Accelerator Architecture

Petr Anisimov
20200287ER



Conventional accelerators achieve electron bunch compression with a help of a large magnetic system called a chicane (top). Such an approach is not suitable for compressing electron bunches for use in high brightness high energy free electron lasers due to microbunching instability inherent to this approach. The laser assisted bunch compression scheme suppresses the microbunching instability by combining a laser modulation with a much smaller chicane. The advantage of the proposed compression scheme will be demonstrated by a start to end simulation of a high brightness high energy free electron laser.

Project Description

X-ray free-electron lasers (XFELs) are billion-dollar-class scientific instruments used for discovery science in materials, biology, and chemistry, and also for national security applications. For example, Los Alamos has identified an XFEL as a potential tool to address developing a needed future capability for ensuring the viability of the nation's nuclear assets, the dynamic mesoscale materials science capability (DMMSC). Despite their cost, the broad impact of XFELs has led to the recent development of a half-dozen XFEL facilities worldwide, including one already operating in the United States and another coming on-line in a few years. Their high cost results from electron beam instabilities in the accelerators driving the XFELs, which presently can only be mitigated by increasing the electron beam energy. This in turn requires a longer (and more expensive) accelerator. The goal of this project is to investigate if a novel accelerator architecture generating a microbunched electron beam can suppress these instabilities to the point that significantly lower electron beam energies (and thus a much less expensive accelerator) can be used to drive XFELs. If so, this approach may lead to XFELs inexpensive enough that they can become university-laboratory sized tools.

Technical Outcomes

The project has delivered a start-to-end analysis of the proposed accelerator architecture. This analysis has demonstrated successful mitigation of electron beam instabilities in a low energy accelerator envisioned for the dynamic mesoscale materials science capability at Los Alamos National Laboratory. The team has strengthened collaboration with University of California Los Angeles on cryogenically cooled C-band acceleration and university size X-ray free electron lasers.

Publications

Journal Articles

Marksteiner, Q. R., N. Yampolsky, H. Xu, L. D. Duffy, P. M. Anisimov, B. E. Carlsten and J. W. I. Lewellen. Analytical Calculations of the Energy Spread Induced by the Microbunching Instability. Submitted to *Intended for publication in Physical Review Accelerators and Beams*. (LA-UR-22-31568)

*Rosenzweig, J. B., N. Majernik, R. R. Robles, G. Andonian, O. Camacho, A. Fukasawa, A. Kogar, G. Lawler, J. Miao, P. Musumeci, B. Naranjo, Y. Sakai, R. Candler, B. Pound, C. Pellegrini, C. Emma, A. Halavanau, J. Hastings, Z. Li, M. Nasr, S. Tantawi, P. Anisimov, B. Carlsten, F. Krawczyk, E. Simakov, L. Faillace, M. Ferrario, B. Spataro, S. Karkare, J. Maxson, Y. Ma, J. Wurtele, A. Murokh, A. Zholents, A. Cianchi, D. Cocco and S. B. van der Geer. An ultra-compact x-ray free-electron laser. 2020. *New Journal of Physics*. **22** (9): 93067. (LA-UR-20-29584 DOI: 10.1088/1367-2630/abb16c)

Xu, H., B. E. Carlsten, L. D. Duffy, Q. R. Marksteiner, P. M. Anisimov and R. R. Robles. X-ray Free Electron Laser Accelerator Lattice Design Using Laser-Assisted Bunch Compression. 2023. *Applied Sciences*. **13** (4): 2285. (LA-UR-22-24776 DOI: 10.3390/app13042285)

Conference Papers

Marksteiner, Q. R., P. M. Anisimov, B. E. Carlsten, G. Latour, E. I. Simakov and H. Xu. Suppressing the Microbunching Instability at ATF using Laser Assisted Bunch Compression. Presented at *North American Particle Accelerator Conference (NAPAC)*. (Albuqueque, New Mexico, United States, 2022-08-08 - 2022-08-12). (LA-UR-22-28054)

Xu, H., L. D. Duffy, Q. R. Marksteiner and P. M. Anisimov. comparison study on first bunch compressor schemes by conventional and double C-chicane for MaRIE XFEL. Presented at *North American Particle Accelerator Conference (NAPAC)*. (Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12). (LA-UR-22-26792)

Presentation Slides

Anisimov, P. M., D. C. Nguyen and N. Neveu. Time-independent 3D FEL Simulations. . (LA-UR-21-20607)

Anisimov, P. M., D. C. Nguyen and N. Neveu. Time-dependent 3D FEL Simulations. . (LA-UR-21-20803)

Anisimov, P. M., N. Neveu and D. C. Nguyen. Introduction to FEL Simulations. . (LA-UR-21-20608)

Carlsten, B. E. Accelerator technology studies for X-ray FELs. . (LA-UR-21-27087)

Marksteiner, Q. R., P. M. Anisimov, B. E. Carlsten, G. Latour, E. I. Simakov and H. Xu. Suppressing the Microbunching Instability at ATF using Laser Assisted Bunch Compression. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-08 - 2022-08-12. (LA-UR-22-28060)

Neveu, N., P. M. Anisimov and D. C. Nguyen. Optimization and Beam Shaping. . (LA-UR-21-21188)

Nguyen, D. C., P. M. Anisimov, Y. Li and N. Neveu. Self-Seeding, Regenerative Amplifier FEL & XFELO. . (LA-UR-21-21184)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Introduction, Electron Motions in an Undulator, Undulator Radiation & FEL. . (LA-UR-21-20610)

Nguyen, D. C., P. M. Anisimov and N. Neveu. SASE, High-Gain FEL & 1D Theory. . (LA-UR-21-20609)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Harmonic Generation, HGHG & EEHG. . (LA-UR-21-21185)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Electron Bunch Compression, CSR, mBi, Laser Heater & Machine Layout. . (LA-UR-21-21190)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Photoinjectors, Emittance Revisited, Photoinjector Design & Optimization. . (LA-UR-21-21187)

Posters

Xu, H., B. E. Carlsten, L. D. Duffy, Q. R. Marksteiner and P. M. Anisimov. Comparison study on first bunch compressor schemes by conventional and double C-chicane for MaRIE XFEL. Presented at *North American Particle Accelerator Conference (NAPAC)*, Albuquerque, New Mexico, United States, 2022-08-07 - 2022-08-12. (LA-UR-22-27892)

**Peer-reviewed*

MixIT – Understanding Mix in Fusion Implosions Through Ion Temperature Imaging

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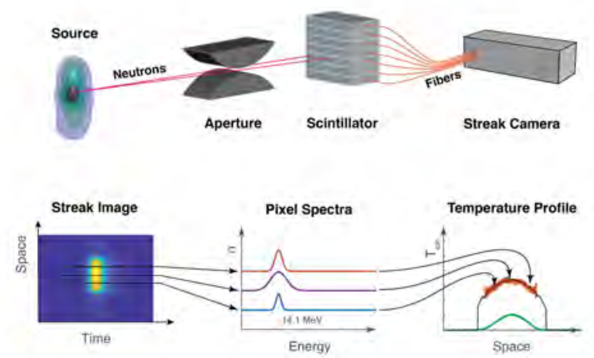

MixIT will produce the first-ever spatially resolved ion temperature measurement of inertial confinement fusion (ICF) implosions. A cleverly designed instrument using a thick neutron aperture and a segmented scintillator projects a neutron image onto a streak camera, providing time resolution (see detector schematic in top panel). This time resolution allows for time-of-flight determination of the neutron energy which is correlated to ion temperature by thermal broadening of the neutron energy distribution for each spatial bin – leading to the first ion temperature measurement that preserves spatial information (bottom panel).

Project Description

This project will produce the first-ever spatially resolved ion temperature measurement of inertial confinement fusion (ICF) implosions. The novel measurement has the potential to uncover the missing piece on the path to ignition for future fusion facilities. Leveraging our expertise as world leaders in fusion neutron imaging we will enhance cutting-edge technology to determine plasma ion temperature – adding a transformational diagnostic capability to Los Alamos National Laboratory's toolkit for fusion research. The injection of contaminant mass into fuel regions - or mix - is believed to be a primary factor preventing ignition at the National Ignition Facility - the world's most powerful ICF facility. Knowledge of the temperature distribution in the hot spot will be crucial for determining accurate estimates of the amount of contaminant and for providing constraints on radiation-hydrodynamics modeling of ICF experiments. A better understanding of ICF burn and hydrodynamic mix does not only advance the United States fusion program, it also ties directly into our core mission of stockpile stewardship.

Technical Outcomes

The team has successfully measured an inertial confinement fusion temperature profile by developing and fielding a brand-new diagnostic. A neutron imaging diagnostic was designed with a model-based approach, and the system was successfully fielded at the OMEGA Laser Facility. Analyses of the captured data have resulted in the achievement of the project goal: measurement of the first-ever spatially resolved ion temperature profile for ICF.

Publications

Journal Articles

Birge, N., V. Geppert-Kleinrath, C. Danly, B. Haines, S. T. Ivancic, J. Jorgenson, J. Katz, E. Mendoza, A. T. Sorce, L. Tafoya, C. Wilde and P. Volegov. Instrument design for an inertial confinement fusion ion temperature imager. 2022. *Review of Scientific Instruments*. **93** (11): 113510. (LA-UR-22-25199 DOI: 10.1063/5.0101820)

Danly, C. R., N. W. Birge, V. Geppert-Kleinrath, B. M. Haines, S. T. Ivancic, H. J. Jorgenson, J. Katz, F. E. Merrill, E. F. Mendoza, A. Sorce, L. R. Tafoya, P. L. Volegov, C. H. Wilde and D. C. Wilson. Development of a spatially-resolved ion temperature diagnostic for inertial confinement fusion. Submitted to *Review of Scientific Instruments*. (LA-UR-22-25849)

Presentation Slides

Birge, N. W., V. Geppert-Kleinrath, C. R. Danly, B. M. Haines, H. J. Jorgenson, E. F. Mendoza, L. R. Tafoya, P. L. Volegov and C. H. Wilde. MixIT: designing a 1D ion temperature imager for ICF. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30939)

Birge, N. W., V. Geppert-Kleinrath, C. R. Danly, P. L. Volegov, C. H. Wilde and B. M. Haines. Photometrics for the MixIT Project. . (LA-UR-20-27133)

Birge, N. W., V. Geppert-Kleinrath, C. R. Danly, V. E. Fatherley, M. S. Freeman, H. J. Jorgenson, E. F. Mendoza, L. R. Tafoya, C. H. Wilde, P. Younk, K. T. Hughes and D. Fittinghoff. Extending neutron imaging capabilities for Inertial Confinement Fusion. . (LA-UR-22-25848)

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Geppert-Kleinrath, V. The Quest for Symmetry:\xc2\xa03D Nuclear Imaging of Inertial Confinement Fusion \xc2\xa0Implosions. Presented at *Laboratory for Laser Energetics, University of Rochester Seminar*, Rochester, New York, United States, 2021-12-10 - 2021-12-10. (LA-UR-21-32155)

Geppert-Kleinrath, V., P. L. Volegov, C. R. Danly, N. W. Birge, C. H. Wilde and B. M. Haines. MixIT – Understanding Mix in Fusion Implosions through Ion Temperature Imaging. Presented at *Physics Cafe*, Los Alamos, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-23206)

Mendoza, E. F., V. Geppert-Kleinrath, N. W. Birge and C. R. Danly. MCNP Simulations for Aperture Alignment In ICF Imaging. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27640)

Posters

Birge, N. W., C. R. Danly, V. Geppert-Kleinrath, B. M. Haines, H. J. Jorgenson, E. F. Mendoza, L. R. Tafoya, C. H. Wilde, J. Katz, S. T. Ivancic and A. T. Sorce. Instrument design for an ICF ion temperature imager. Presented at *Conference on High Temperature Plasma Diagnostics (HTPD)*, Rochester, New York, United States, 2022-05-16 - 2022-05-20. (LA-UR-22-24261)

**Peer-reviewed*

The Missing Link: Quantum Mechanics in Plasma Kinetic Modeling

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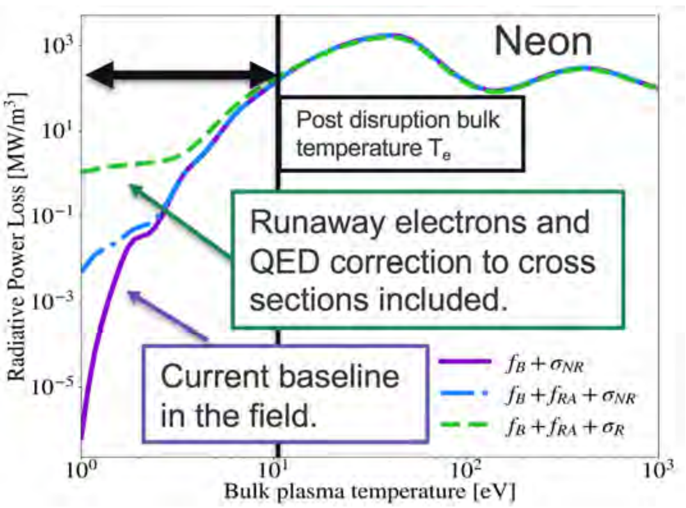

The tokamak disruption problem poses a serious threat to the future success of International Thermonuclear Experimental Reactor (ITER) and efficiently harnessing magnetic fusion energy. During a disruption event relativistic runaway electrons are generated, and neon is injected to promote the cooling of runaway electrons. Our goal is to bring accurate atomic physics to the plasma modeling of such scenarios. The purple line is the current physics used in the field only accounting for the bulk thermal electrons, while the green line shows the developments made here and the effect of the relativistic runaway electrons on the plasma cooling.

Project Description

The tokamak disruption problem poses a serious threat to the future success of the International Thermonuclear Experimental Reactor (ITER), efficiently harnessing magnetic confinement nuclear fusion energy, and understanding energy production in civilian applications. During this project we will develop the Los Alamos atomic physics suite of codes to support the plasma modeling effort to design a tokamak disruption mitigation system. Los Alamos is the ideal venue for such research, as this problem requires a cross-disciplinary synergistic approach between atomic physicists, and plasma physicists, as well as the utilization of abundant computing resources and sophisticated atomic physics tools that are only available at Los Alamos. This project will contribute to the design and implementation of a disruption mitigation system that is required in the operations of ITER and future fusion tokamak facilities.

The developments made during this project will have a direct application to inertial confinement fusion experiments.

Technical Outcomes

The project was a success, with the Los Alamos National Laboratory atomic physics suite of codes developed to calculate comprehensive sets of collision data for modeling fusion plasmas. The developments and results of this project have left Los Alamos National Laboratory in a leadership position for calculating the collision data and models required for plasma modeling applications.

Publications

Journal Articles

*Garland, N. A., H. Chung, C. J. Fontes, M. C. Zammit, J. Colgan, T. Elder, C. J. McDevitt, T. M. Wildey and X. Tang. Impact of a minority relativistic electron tail interacting with a thermal plasma containing high-atomic-number impurities. 2020. *Physics of Plasmas*. **27** (4): 040702. (LA-UR-19-28749 DOI: 10.1063/5.0003638)

*Garland, N. A., H. Chung, M. C. Zammit, C. J. McDevitt, J. Colgan, C. J. Fontes and X. Tang. Understanding how minority relativistic electron populations may dominate charge state balance and radiative cooling of a post-thermal quench tokamak plasma. 2022. *Physics of Plasmas*. **29** (1): 012504. (LA-UR-21-29190 DOI: 10.1063/5.0071996)

*Garland, N. A., H. Chung, M. C. Zammit, C. J. McDevitt, J. Colgan, C. J. Fontes and X. Tang. Understanding how minority relativistic electron populations may dominate charge state balance and radiative cooling of a post-thermal quench tokamak plasma. 2022. *Physics of Plasmas*. **29** (1): 012504. (LA-UR-21-29190 DOI: 10.1063/5.0071996)

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Horton, R. K., D. V. Fursa, L. H. Scarlett, I. Bray and M. C. Zammit. Electron energy deposition in molecular hydrogen gas: a Monte-Carlo simulation using convergent close-coupling cross sections. Submitted to *Plasma Sources Science and Technology*. (LA-UR-21-26392)

Mori, N. A., R. Utamuratov, D. V. Fursa, M. C. Zammit and I. Bray. Calculation of the single differential cross section for electron-impact ionization of atoms and molecules. Submitted to *Physical Review A*. (LA-UR-20-23099)

Padovani, M., S. Bialy, D. Galli, A. Ivlev, T. Grassi, L. H. Scarlett, U. Rehill, M. C. Zammit, D. V. Fursa and I. Bray. Cosmic rays in molecular clouds probed by H2 rovibrational lines Perspectives for the James Webb Space Telescope. Submitted to *Astronomy and Astrophysics*. (LA-UR-21-29186)

Park, R. M., W. R. Kupets, M. C. Zammit, J. P. Colgan, C. J. Fontes, B. S. Scheiner, E. M. E. Timmermans, X. Tang, L. H. Scarlett, D. V. Fursa, I. Bray and N. A. Garland. Anisotropic angular scattering models of elastic electron-neutral collisions for Monte Carlo plasma simulations. Submitted to *Plasma Sources Science & Technology*. (LA-UR-21-32313)

Scarlett, L. H., D. K. Boyle, M. C. Zammit, Y. Ralchenko, I. Bray and D. V. Fursa. Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues: III. Vibrational excitation via electronic excitation and radiative decay. 2022. *Atomic Data and Nuclear Data Tables*. 101534. (LA-UR-22-22070 DOI: 10.1016/j.adt.2022.101534)

Scarlett, L. H., D. V. Fursa, J. Knol, M. C. Zammit and I. Bray. Isotopic and vibrational-level dependence of H2 dissociation by electron impact. Submitted to *Physical Review A*. (LA-UR-20-29938)

Scarlett, L. H., E. Jong, S. Odelia, M. C. Zammit, Y. Ralchenko, B. I. Schneider, I. Bray and D. V. Fursa. Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues: IV. Vibrationally-resolved ionization of the ground and excited electronic states. 2023. *Atomic Data and Nuclear Data Tables*. 101573. (LA-UR-22-29219 DOI: 10.1016/j.adt.2023.101573)

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Garland, N. A., R. Maulik, Q. Tang, X. Tang and P. Balaprakash. Progress towards high fidelity collisional-radiative model surrogates for rapid in-situ evaluation. Presented at *Machine Learning and the Physical Sciences Workshop at the 34th Conference on Neural Information Processing Systems (NeurIPS)*. (Virtual (originally Vancouver), Canada, 2020-12-11 - 2020-12-11). (LA-UR-20-28192)

Reports

George, A., M. C. Zammit and N. A. Garland. Summer 2020 Los Alamos National Laboratory Report. Unpublished report. (LA-UR-21-24169)

George, A., M. C. Zammit and N. A. Garland. Summer 2020 Los Alamos National Laboratory Report. Unpublished report. (LA-UR-21-24169)

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2021, Virtual, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25163)

Colgan, J. P., M. C. Zammit, N. A. Garland, J. Li, C. J. Fontes, X. Tang and M. S. Pindzola. Angular distributions for electron-impact ionization of noble gases and their application to plasma modeling. Presented at *DAMOP 2020*, Portland, Oregon, United States, 2020-06-02 - 2020-06-02. (LA-UR-20-24064)

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Garland, N. A., A. George and M. C. Zammit. Uncertainty quantification of atomic data for collisional-radiative modeling of fusion plasmas. Presented at *LANL T-Div Student Lightning talks*, Los Alamos, New Mexico, United States, 2020-08-04 - 2020-08-04. (LA-UR-20-25815)

Garland, N. A., M. C. Zammit, C. J. Fontes, J. P. Colgan, H. K. Chung and X. Tang. A collisional-radiative model benchmarking and comparative study of fusion relevant atoms. Presented at *GEC 2020*, San Diego, California, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-28191)

George, A., N. A. Garland and M. C. Zammit. Collisional Radiative model for nuclear fusion. . (LA-UR-20-24941)

George, A., W. R. Kupets, N. A. Garland and M. C. Zammit. Uncertainty quantification of atomic data for collisional-radiative modeling of fusion plasmas. . (LA-UR-21-24165)

George, A., W. R. Kupets, N. A. Garland and M. C. Zammit. Uncertainty quantification of atomic data for collisional-radiative modeling of fusion plasmas. . (LA-UR-21-24165)

Kupets, W. R., N. A. Garland, J. P. Colgan, C. J. Fontes, X. Tang, I. Bray, D. V. Fursa, L. H. Scarlett and M. C. Zammit. Comparisons and fits of electron angular distribution approximations for elastic scattering from neutral fusion-relevant targets. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Virtual Conference, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25045)

Kupets, W. R., N. A. Garland, J. P. Colgan, C. J. Fontes, X. Tang, I. Bray, D. V. Fursa, L. H. Scarlett and M. C. Zammit. Comparisons and fits of electron angular distribution approximations for elastic scattering from neutral fusion-relevant targets. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Virtual Conference, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25045)

Park, R. M., M. C. Zammit, B. S. Scheiner, J. P. Colgan, C. J. Fontes, E. M. E. Timmermans, X. Tang and N. A. Garland. A General Analytic Electron Energy Sharing Distribution for Monte-Carlo Plasma Codes. . (LA-UR-22-27797)

Park, R. M., M. C. Zammit, B. S. Scheiner, J. P. Colgan, C. J. Fontes, E. M. E. Timmermans, X. Tang and N. Garland. A General Analytic Electron-Impact Ionization Electron Energy Sharing Model for Monte Carlo Plasma and Swarm Applications. Presented at *Annual Gaseous Electronics Conference*, Sendai, Japan, 2022-10-03 - 2022-10-07. (LA-UR-22-29986)

Park, R. M., M. C. Zammit, W. R. Kupets, J. P. Colgan, C. J. Fontes, X. Tang, L. H. Scarlett, D. V. Fursa, I. Bray and N. A. Garland. LOW-TEMPERATURE PLASMA TRANSPORT COEFFICIENTS DERIVED FROM SCATTERING ANGULAR DISTRIBUTION FUNCTIONS. . (LA-UR-21-27525)

Sanchez, J. T., M. C. Zammit, J. P. Colgan and C. J. Fontes. Benchmark Collisional-Radiative Modeling of Fusion-Relevant Plasmas. . (LA-UR-22-27388)

Zammit, M. C. Elastic scattering angular distribution function model for H, He and H2: Impact on modeling swarm data. . (LA-UR-22-24980)

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Zammit, M. C., J. P. Colgan, C. J. Fontes, N. A. Garland, J. C. A. O. Jung, A. J. Neukirch, R. M. Park, B. S. Scheiner, X. Tang and E. M. E. Timmermans. Electron Collision Models and Data for Kinetic Modeling. . (LA-UR-22-30728)

Zammit, M. C., J. P. Colgan, D. P. Kilcrease, C. J. Fontes, P. Hakel, J. A. Leiding, J. C. A. O. Jung, E. M. E. Timmermans, J. S. Savage, D. V. Fursa, A. S. Kadyrov, I. Bray, M. Charlton, S. Jonsell and R. C. Forrey. Molecular Data for Atmospheric Physics, Plasma Modeling and Antimatter Molecule Production. Presented at *GEM XXI ATMOP 2020*, Canberra, Australia, 2020-02-11 - 2020-02-11. (LA-UR-20-21966)

Zammit, M. C., J. P. Colgan, D. P. Kilcrease, C. J. Fontes, P. Hakel, J. A. Leiding, J. C. A. O. Jung, E. M. E. Timmermans, J. S. Savage, D. V. Fursa, A. S. Kadyrov, I. Bray, M. Charlton, S. Jonsell and R. C. Forrey. Molecular Data for Atmospheric Physics, Plasma Modeling and Antimatter Molecule Production. . (LA-UR-20-22047)

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Zammit, M. C., J. P. Colgan, R. M. Park, C. J. Fontes, B. S. Scheiner, E. M. E. Timmermans, X. Tang and N. A. Garland. An Analytic Electron-Impact Ionization Anisotropic Scattering Model for Monte Carlo Plasma. Presented at *64th Annual Meeting of the APS Division of Plasma Physics*, Spokane, Washington, United States, 2022-10-17 - 2022-10-17. (LA-UR-22-30887)

Zammit, M. C., J. P. Colgan, R. M. Park, C. J. Fontes, B. S. Scheiner, E. M. E. Timmermans, X. Tang and N. Garland. An Analytic Electron-Impact Ionization Anisotropic Scattering

Model for Monte Carlo Plasma and Swarm Applications. Presented at *Annual Gaseous Electronics Conference*, Sendai, Japan, 2022-10-03 - 2022-10-03. (LA-UR-22-30035)

Zammit, M. C., N. A. Garland, W. R. Kupets, J. P. Colgan, C. J. Fontes, J. Li and X. Tang. FY20 Appraisal: The Missing Link? Quantum Mechanics in Plasma Kinetic Modeling. . (LA-UR-20-29400)

Zammit, M. C., N. A. Garland, W. R. Kupets, R. M. Park, J. P. Colgan, C. J. Fontes and X. Tang. FY21 Appraisal: The Missing Link? Quantum Mechanics in Plasma Kinetic Modeling. . (LA-UR-22-20060)

Zammit, M. C., R. M. Park, W. R. Kupets, J. P. Colgan, C. J. Fontes, B. S. Scheiner, E. M. E. Timmermans, X. Tang, L. H. Scarlett, D. V. Fursa, I. Bray and N. A. Garland. Anisotropic Elastic Scattering Models of Neutral Fusion-Relevant Species for Monte Carlo Plasma Modeling. Presented at *64th Annual Meeting of the APS Division of Plasma Physics*, Spokane, Washington, United States, 2022-10-17 - 2022-10-17. (LA-UR-22-30838)

Posters

Park, R. M., M. C. Zammit, B. S. Scheiner, J. P. Colgan, C. J. Fontes, E. M. E. Timmermans, X. Tang and N. Garland. A General Analytic Electron-Impact Ionization Electron Energy Sharing Model for Monte Carlo Plasma Modeling. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30829)

Sanchez, J. T., M. C. Zammit, C. J. Fontes, J. P. Colgan, N. A. Garland and X. Tang. Benchmark Collisional-Radiative Modeling of Magnetic Fusion-Relevant Plasmas. Presented at *64th Annual Meeting of the APS Division of Plasma Physics*, Spokane, Washington, United States, 2022-10-17 - 2022-10-17. (LA-UR-22-30825)

**Peer-reviewed*

How do Pulsar Winds Shine in Tera Electron Volt (TeV)?

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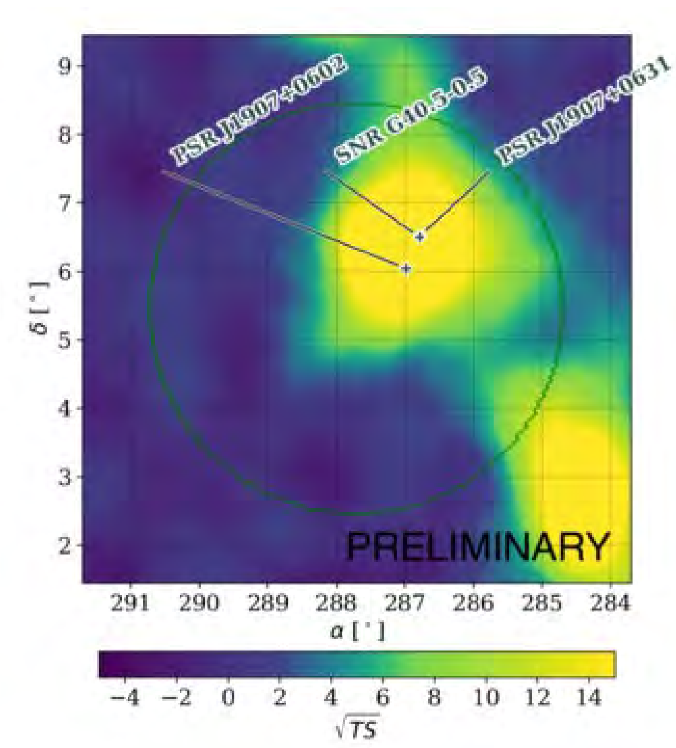
20200367ER



The project aims to perform theoretical modeling and observations to pin down particle acceleration processes in Tera Electron Volt (TeV) pulsar wind nebulae. The figure is a gamma-ray image of HAWC observation of J1908+63 (HAWC collaboration).

Project Description

This project aims at understanding the origin of multi-Tera Electron Volt (TeV) emission from pulsar wind nebulae powered by termination shocks created by relativistic pulsar winds. This is a fundamental question in our understanding of the cosmos. This project brings together theory, numerical modeling, and multi-wavelength observations including gamma-rays. It builds capabilities in particle and gamma-ray detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Technical Outcomes

Using a newly developed algorithm, the team found a Fermi acceleration mechanism operating at the termination shock of pulsar wind nebulae and enabling the acceleration to ~100 tera electron Volts. The detailed radiation model and optimized data analysis show that the pulsar wind spectrum cannot be explained by a single electron population, which may indicate a high-energy hadronic component. The project led to new advances in understanding particle acceleration and high-energy emissions in pulsar winds.

Publications

Journal Articles

*Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. T. Dahlin, B. Chen, G. Fleishman, L. Glesener, E. Kontar, T. Phan and C. Shen. Electron Acceleration during Macroscale Magnetic Reconnection. 2021. *Physical Review Letters*. **126** (13): 135101. (LA-UR-20-30073 DOI: 10.1103/PhysRevLett.126.135101)

*Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. T. Dahlin and Q. Zhang. Slow Shock Formation Upstream of Reconnecting Current Sheets. 2022. *The Astrophysical Journal*. **926** (1): 24. (LA-UR-21-27254 DOI: 10.3847/1538-4357/ac423b)

*Chen, Q., K. Nalewajko and B. Mishra. Scaling of magnetic dissipation and particle acceleration in ABC fields. 2021. *Journal of Plasma Physics*. **87** (2): 905870224. (LA-UR-21-20632 DOI: 10.1017/S0022377821000209)

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Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated Particle Acceleration in the Presence of Ambient Solar-Wind Turbulence. 2021. *Frontiers in Astronomy and Space Sciences*. **8**: 644354. (LA-UR-20-30411 DOI: 10.3389/fspas.2021.644354)

*Guo, F., X. Li, W. Daughton, H. Li, P. Kilian, Y. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics, and Particle Acceleration in Relativistic Turbulent Magnetic Reconnection. 2021. *The Astrophysical Journal*. **919** (2): 111. (LA-UR-20-26005 DOI: 10.3847/1538-4357/ac0918)

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Harding, A. K. and C. Venter. Very-High-Energy Emission From Pulsars. Submitted to *Astrophysical Journal*. (LA-UR-21-30389)

*Harding, A. K. and G. Younes. Broadband X-ray burst spectroscopy of the fast-radio-burst-emitting Galactic magnetar. 2021. *Nature Astronomy*. **5** (4): 408-413. (LA-UR-21-22817 DOI: 10.1038/s41550-020-01292-x)

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*Kilian, P., X. Li, F. Guo and H. Li. Exploring the Acceleration Mechanisms for Particle Injection and Power-law Formation during Transrelativistic Magnetic Reconnection. 2020. *The Astrophysical Journal*. **899** (2): 151. (LA-UR-20-20135 DOI: 10.3847/1538-4357/aba1e9)

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Kong, X., J. Ye, B. Chen, F. Guo, C. Shen, X. Li, S. Yu, Y. Chen and J. Giacalone. A model of double coronal hard X-ray sources in solar flares. Submitted to *Astrophysical Journal*. (LA-UR-22-25675)

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*Zhang, H., X. Li, D. Giannios and F. Guo. First-principles Prediction of X-Ray Polarization from Magnetic Reconnection in High-frequency BL Lacertae Objects. 2021. *The Astrophysical Journal*. **912** (2): 129. (LA-UR-20-30074 DOI: 10.3847/1538-4357/abf2be)

*Zhang, Q., F. Guo, W. Daughton, H. Li and X. Li. Efficient Nonthermal Ion and Electron Acceleration Enabled by the Flux-Rope Kink Instability in 3D Nonrelativistic Magnetic Reconnection. 2021. *Physical Review Letters*. **127** (18): 185101. (LA-UR-21-24459 DOI: 10.1103/PhysRevLett.127.185101)

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Durocher, M. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *APS April 2021*, Washington, District Of Columbia, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23269)

Durocher, M. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30472)

Durocher, M. Limits on Diffuse Dark Matter with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30475)

Durocher, M. Searching for the Diffuse Gamma-Ray Background with HAWC. . (LA-UR-21-30456)

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Durocher, M. Limits on Diffuse Dark Matter with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30451)

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Guo, F. First Principles Kinetic Simulations of Relativistic Collisionless Shocks and Their Particle Acceleration. . (LA-UR-20-25828)

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H. Kilian, P. F. Numerical Plasma Physics. . (LA-UR-20-23604)

H. Kilian, P. F., X. Li, F. Guo and H. Li. How magnetic reconnection injects particles and accelerates them to high energies. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-22043)

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Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25532)

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Malone, K. A., K. Mori, B. L. Dingus, H. An, C. J. Hailey, B. Humensky, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR X-ray observation campaign of energetic pulsar wind nebulae. Presented at *International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-26302)

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Durocher, M. Limits on Diffuse Dark Matter with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30453)

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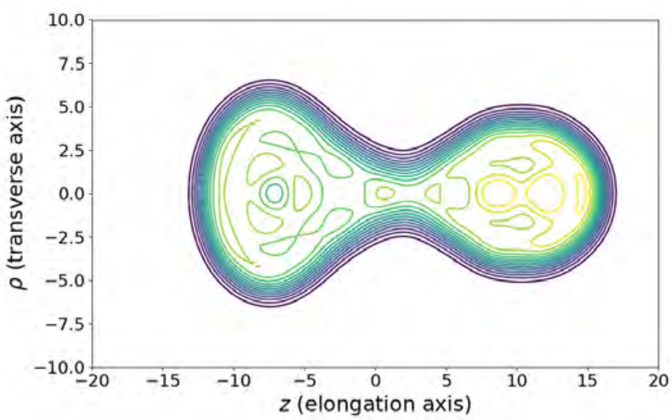
**Peer-reviewed*

A Dynamical Approach to Low-Energy Fission

Matthew Mumpower
20200384ER



The density of nucleons of the fissioning system 236-U (uranium 236) right as the nucleus breaks apart into two fragments. This LDRD supported project on fission dynamics greatly improves the description of the resultant fragments.

Project Description

Fission yields are important for a variety of applications and for our basic scientific understanding of the fission process and many-body nuclear physics. For nonproliferation purposes, fission fragments represent the initial conditions that decide upon the emission of neutron and gamma emission, which constitute signatures of specific nuclear materials. For nuclear forensics, fission yields are needed to identify the fuel and determine the neutron spectra that can be used to reconstruct and infer specific designs. For stockpile stewardship, fission yields are also needed to interpret historical data. For nuclear energy and nuclear waste management purposes, fission yields are needed in a large range of applications, like decay heat, shielding, dosimetry, fuel handling and safe waste disposal. They are also critical to properly perform a fission product inventory at each stage of the nuclear fuel cycle in reactors. Other applications include safeguards for nuclear reactor monitoring and medical applications for radioisotope production. This work is directed at improving the modeling capabilities needed in such applications, by implementing state-of-the art theoretical models capable of producing fission yields to be used in a variety of applications.

Technical Outcomes

The project was successful in its goal of studying low-energy fission dynamics for the major actinides. The team calculated new potential energy surfaces for major actinides. The team delivered a new framework for fission transport that supports three increasing levels of sophistication: (1) Brownian shape motion, (2) Smoluchowski dynamics and (3) Langevin dynamics. Finally the team compared their new fission simulations with precision measurements and found that the models with increased sophistication had optimal performance.

Publications

Journal Articles

*Bulgac, A., I. Abdurrahman, K. Godbey and I. Stetcu. Fragment Intrinsic Spins and Fragments' Relative Orbital Angular Momentum in Nuclear Fission. 2022. *Physical Review Letters*. **128** (2): 022501. (LA-UR-21-27848 DOI: 10.1103/PhysRevLett.128.022501)

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Mumpower, M. R., T. M. Sprouse, T. Kawano, M. W. Herman, A. E. Lovell, G. W. Misch, D. Neudecker, H. Sasaki, I. Stetcu and P. Talou. Nuclear data activities for medium mass and heavy nuclei at Los Alamos. Presented at *International Conference on Nuclear Data for Science and Technology*. (Sacramento, California, United States, 2022-07-24 - 2022-07-29). (LA-UR-22-30993)

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Mumpower, M. R. KISS-II Review. . (LA-UR-22-20418)

Mumpower, M. R., I. Stetcu and T. M. Sprouse. A Dynamical Approach to Low-Energy Fission. . (LA-UR-21-31795)

Sprouse, T. M. Propagation of nuclear model uncertainties in science applications. Presented at *Workshop for Applied Nuclear Data Activities*, Los Alamos (virtual via WebEx), New Mexico, United States, 2021-01-25 - 2021-02-03. (LA-UR-21-20577)

Sprouse, T. M. Connecting nuclear isomers with nuclear astrophysics: current status and future needs. Presented at *Low Energy Community Meeting 2022*, Chicago, Illinois, United States, 2022-08-08 - 2022-08-10. (LA-UR-22-28282)

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Posters

Sprouse, T. M., M. R. Mumpower and I. Stetcu. Towards a Langevin Model for the Stochastic Dynamics of Nuclear Fission. Presented at *International Conference on Nuclear Data for Science and Technology*, Los Alamos (Virtual), New Mexico, United States, 2022-07-24 - 2022-07-29. (LA-UR-22-26926)

Other

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**Peer-reviewed*

Development of Superconducting Accelerating Cavities with Magnesium Diboride (MgB2) Coating

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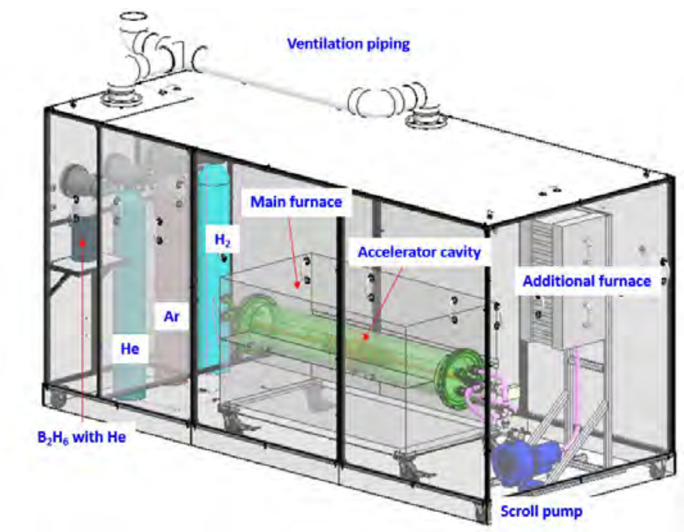
20210720ER



The project investigates optimum coating parameters to yield a high-quality magnesium diboride (MgB2) superconductor. The diagram shows a three-dimensional model of the new MgB2 coating system. A 1.3-gigahertz accelerator cavity will be coated with MgB2 in two steps, coating of boron using diborane gas and then react it with magnesium at 300-400 celsius and ~700 celsius, respectively. It has an additional heater to completely decompose toxic diborane gas and ventilation system for safety.

Project Description

This project will develop a technique to coat a particle accelerator structure with magnesium diboride (MgB2) , a promising superconductor that has a great potential to reduce the size and construction cost compared to the accelerator based on the conventional superconductor niobium (Nb) since it can become superconductive at a >4 times higher temperature (39 Kelvin vs. 9 Kelvin). If successful, an MgB2 coated accelerator can be a small module with a small cooler so-called a cryocooler instead of using liquid helium that requires a large facility to re-liquefy the evaporated helium and circulate the liquid. This compact MgB2 accelerator could be used for various national security missions such space missions, active interrogation for border security, and upgrades of the Los Alamos Neutron Science Center (LANSCE) accelerator for stockpile stewardship. In addition, it can provide an economic solution to the envisioned x-ray free-electron laser based on a high-energy electron accelerator as a part of future Dynamic Mesoscale Materials Science Capability (DMMSC) for Department of Energy / National Nuclear Security Administration.

Technical Outcomes

The project built a new system designed to coat an accelerator cavity. The system had most major components, although the plumbing to coat a boron layer is incomplete. The team started experiments on the reaction of existing boron (B) samples attached on full-size accelerator cavity sample holes with magnesium (Mg) vapor which was not successful due to too low of temperature. The project attained follow-on funding through the Department of Energy, continuing the research.

Publications

Conference Papers

Pizzol, P., I. Nekrashevich, L. Civale, A. Poudel, H. R. Salazar, D. Kelly, R. K. Schulze and T. Tajima. PROGRESS OF MgB2 DEPOSITION TECHNIQUE FOR SRF CAVITIES AT LANL. Presented at *SRF 2021*. (Grand Rapids, Michigan, United States, 2021-06-28 - 2021-07-02). (LA-UR-21-25776)

Presentation Slides

Tajima, T., T. P. Grumstrup, M. A. Mealy, L. Civale, R. K. Schulze, H. R. Salazar, H. Sakai, T. Okada, E. Kako, H. Ito, K. Umemori, D. Kelly, P. Pizzol and A. Poudel. A New System for MgB2 coating R&D at LANL. Presented at *10th International Workshop on Thin Films and New Ideas for Pushing the Limits of RF Superconductivity*, Newport News, Virginia, United States, 2022-09-19 - 2022-09-23. (LA-UR-22-29668)

Posters

Pizzol, P., A. Poudel, I. Nekrashevich, L. Civale, D. Kelly, R. K. Schulze and T. Tajima. PROGRESS OF MgB2 DEPOSITION TECHNIQUE FOR SRF CAVITIES AT LANL. Presented at *SRF 2021*, Grand Rapids, Michigan, United States, 2021-06-28 - 2021-07-02. (LA-UR-21-25818)

**Peer-reviewed*

Studying Double Neutron Capture for Forensics Applications

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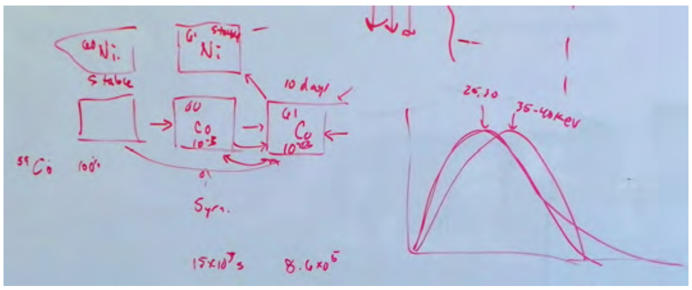


Neutrons produced in nuclear explosions can change the composition of surrounding material, often producing long-lived radioactive species that can be measured after the fact. Subtle changes in the neutron exposure can impact which isotopes are produced. Unfortunately, many of these reactions on unstable isotopes are not measured. In this calculational study, we will investigate which of these reactions could be studied at the Soreq Applied Research Accelerator Facility (SARAF), and how the SARAF spectrum could impact the results.

Project Description

In the event of a nuclear detonation, it is critical that the United States be positioned to rapidly and accurately determine how the device was designed, an effort broadly known as nuclear forensics. Radioactive traces observable after the detonation can reveal information about both the conditions of the detonation and the materials present in the nuclear device. But the fidelity of those determinations is only as good as our knowledge of the reaction channels. A new measurement facility, the Soreq Applied Research Accelerator Facility, offers the chance to study reactions on unstable isotopes in a combined effort to both make and measure the isotope in one experiment. This effort will study exactly which isotopes could be measured with this new facility, and look at which measurements would be most important to pursue in the coming years to meet our strategic objectives for nuclear forensics.

Technical Outcomes

This project developed tools to determine what future measurements are possible for direct determination of outstanding nuclear data challenges, in particular device assessment cross sections for which there is no other path to direct experimental determination in the next decade. The tools developed can quickly determine measurement feasibility both for the existing Soreq Applied Research Accelerator Facility, its planned high energy upgrades, and any other activation flux of an existing or proposed neutron exposure facility.

Publications

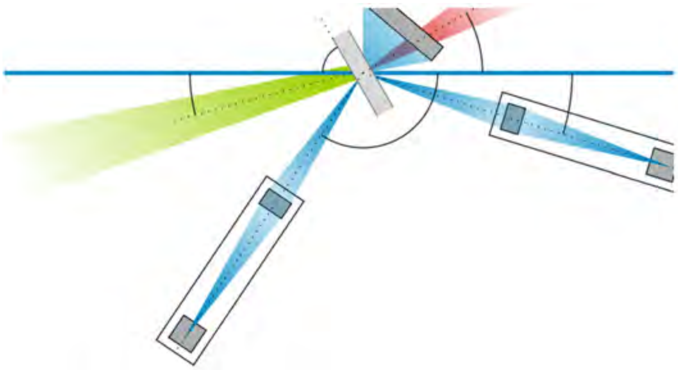
Presentation Slides

Couture, A. J., C. J. Prokop and I. Mardor. LANL/IAEC Collaboration on Nuclear Physics. . (LA-UR-22-23336)

**Peer-reviewed*

Enabling High-Temperature and High-Energy-Density Physics Using X-ray Free Electron Lasers

Steven Batha
20210789ER



A typical configuration for X-ray Thompson Scattering.

Project Description

Ever more precise experiments and measurements must be made to validate the computer simulation codes we use in our national security enterprise. Newly created Department of Energy facilities, such as the fourth-generation light sources, especially the x-ray free electron lasers (XFELs), provide a tremendous advance in the precision that can be attained in certain classes of experiments. This project will develop software that will be used to design experiments so that the accuracy of the measurements can be determined before the experiment is performed. Knowing the uncertainty in the measurements will then quantify the uncertainty in the simulation codes. This will allow for identification of areas where the codes need to be improved. This project will also develop and mature concepts for making large quantities of precision targets that are used to create the experimental conditions, both cheaply and reproducibly.

Technical Outcomes

This project developed tools for designing and executing experiments at the Materials in Extreme Condition instrument at the Linac Coherent Light Source. Simulations showed that spherical targets, rather than flat foils, would make the measurement easier. The project developed a post-processor to predict the spectrum from an x-ray Thomson scattering measurement. Finally, two simple target designs were developed from which a large number of targets could be produced inexpensively.

Publications

Journal Articles

Strickland, A., P. Hakel, N. M. Hoffman and S. H. Batha. Target Design for XFEL Experiments. Submitted to *Fusion Science and Technology*. (LA-UR-22-28558)

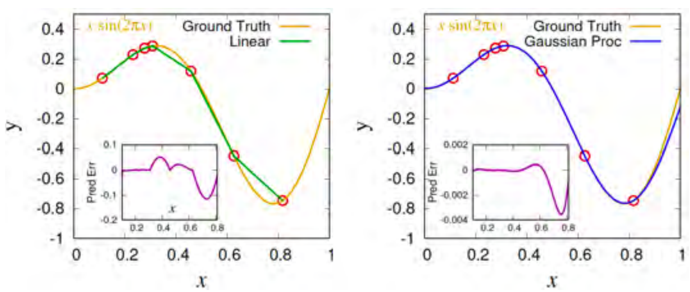
Reports

Batha, S. H., P. Hakel, N. M. Hoffman and A. Strickland. Enabling High-Energy-Density Physics Using X-Ray Free Electron Lasers. Unpublished report. (LA-UR-22-26029)

**Peer-reviewed*

Advancing the Frontiers of High-Precision Quantum Chromodynamics (QCD) with Machine-Learning-Enhanced Monte Carlo Algorithms

Christopher Lee
20210804ER



Discrete approximations to a test integrand in Monte Carlo integration approaches. Left: conventional "linear" interpolation and interpolation errors (inset). Right: new Gaussian interpolation and interpolation errors (inset), two orders of magnitude smaller than linear approach. LANL researchers are implementing this new approach in machine-learning-enhanced algorithms to compute multidimensional integrations in high-energy scattering processes in colliders to probe the strong interaction, structure of protons and hadronic matter, and physics beyond the Standard Model.

Project Description

We apply computational advances based on machine learning to the high-precision prediction of cross sections mediated by the strong interaction in high-energy collisions of electrons, positrons, and protons. Being able to predict the products of these collisions to high accuracy allows them to be used to study the structure of matter and the forces between them in exquisite detail, teaching us about the fundamental nature of matter and evolution of the universe. Our research could enhance the speed and accuracy of computations of these cross sections by factors of 100 or 1000, making a huge impact on the efficiency and range of research on the strong interaction that would be made possible. This would enhance our ability to meet the high-priority scientific goals of the Department of Energy (DOE) Office of Science as expressed in its Long-Range Plans for nuclear science and high-energy physics, to probe the structure of protons, the fundamental forces between their constituents, and search for signs of new physics beyond the Standard Model. It would bolster United States (US) scientific leadership in large international scientific collaborations such as the upcoming Electron-Ion Collider project.

Technical Outcomes

This project contributed to the development of a novel multi-dimensional integration algorithm using machine-learning techniques to efficiently learn and accurately approximate integrands, reducing errors and computational time over classical algorithms. The team also uncovered important discrepancies in key physics software used for Quantum Chromodynamics computations. The discrepancies became apparent only after amassing large statistics made possible by Laboratory high-performance computing.

Publications

Journal Articles

*Yoon, B. A machine learning approach for efficient multi-dimensional integration. 2021. *Scientific Reports*. **11** (1): 18965. (LA-UR-20-27161 DOI: 10.1038/s41598-021-98392-z)

Reports

Lee, C. Final Report Project w21_alphas: Precision determination of the strong coupling in Quantum Chromodynamics. Unpublished report. (LA-UR-22-25152)

Presentation Slides

Lee, C. Gluon radiation from hadronic jets at next-to-next-to-leading order. . (LA-UR-23-23096)

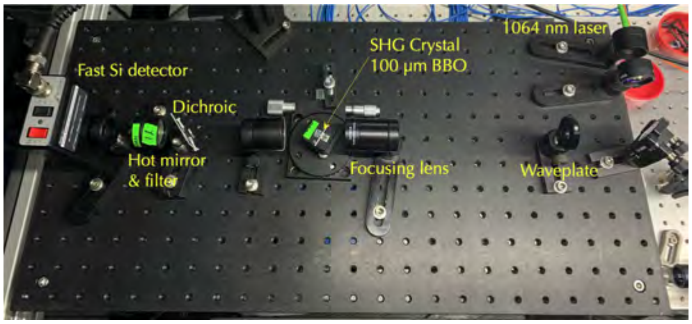
Lee, C., B. Yan, B. Yoon, G. Bell, Y. Makris and J. Talbert. Angularities, gaps, and \\alpha_s. Presented at *World SCET 2021*, Cambridge, Massachusetts, United States, 2021-04-19 - 2021-04-23. (LA-UR-21-23742)

Lee, C., B. Yoon, B. Yan, Y. Makris, J. Talbert and G. Bell. Event shape tails and alpha_s. Presented at *INT Workshop on Probing QCD at High Energy and Density with Jets*, Seattle, Washington, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-27921)

**Peer-reviewed*

Ultrafast Optical Neutron Detector

Kevin Henderson
20210829ER



The image above shows the present experimental setup including the pump laser (>1W 1064nanometers), the second Harmonic generation (SHG) crystal, and a fast detector (~1gigahertz). Future additions to this setup will include homodyne detection for the SHG light and an imaging setup in order to characterize particle detection. This setup should enable detection of actinide alpha decays (e.g., plutonium-239) and ultimately lead to an optical neutron detection capability that is gamma and beta insensitive and does not rely on helium-3.

Project Description

The success of this project could have a big impact on nuclear forensics, characterization of radiation damage, and other programs in Los Alamos National Laboratory (LANL), Department of Energy (DOE), Department of Homeland Security (DHS), and Department of Defense (DOD). But most importantly, this proposed neutron detector is a competitive alternative to Helium-3 neutron detectors which are threatened by a shortage of Helium-3. Alternatives like this proposed detector are especially vital to many DHS and DOE programs.

Technical Outcomes

From the work of this project, a continuous wave detector setup and a separate pulsed experimental setup for surface second harmonic detection were prepared. This project allowed for the experimental framework to be laid out for not just the detection of energetic particles and neutrons but also the characterization of ultrafast changes in materials.

A Search of Weakly-Interacting Dark Matter in the Low Mass Region

Zhaowen Tang
20210834ER

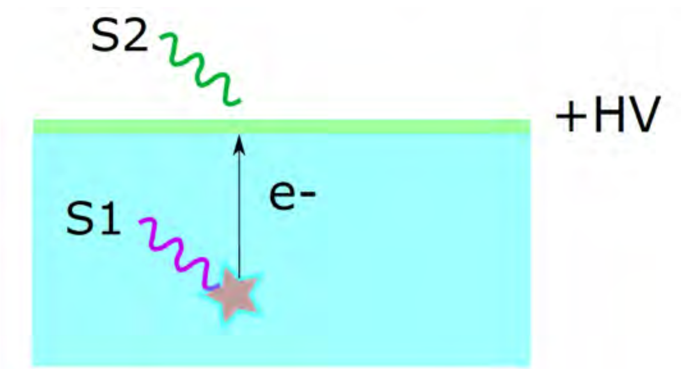


Figure shows the scheme for dark matter detection using p-Terphenyl crystal. A prompt scintillation light is generated from nuclear recoil with the dark matter particle. The electrons from the ionization track generated by the nuclear recoil are accelerated due to the applied voltage, which are then converted to secondary photons by a converter. The development of this new detection scheme can enable us to put constraints on previously unexplored dark matter masses at the sub-giga-electron volt/speed of light (GeV/c^2) regime.

Project Description

Direct detection of dark matter (DM) is an important area of focus for the Department of Energy (DOE) office of science, high energy physics program office. Our dark matter detection idea has a unique opportunity to probe a currently unexplored mass region for both spin independent and spin dependent DM. The result of this project will answer key questions regarding a hydrocarbon-based DM detector, and open up possibility for a prototype experiment that would probe a previously inaccessible parameter space.

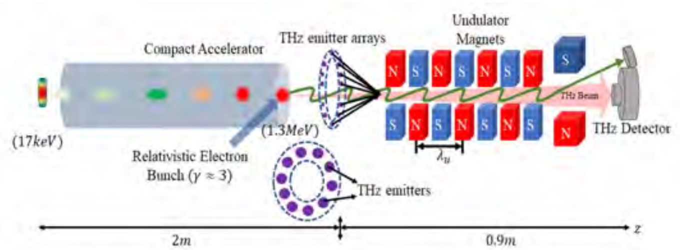
Technical Outcomes

The project team showed that we can extract electrons from p-terphenyl crystals by using an electro-opto conversion material. The work is a proof-of-principle for ionization detecting of the crystal.

Novel Seeding Method for Compact Terahertz (THz) Free Electron Lasers

MD Zuboraj

20210847ER



The project aims to miniaturize a THz Free Electron Laser using a novel seeding method. The figure demonstrates a compact FEL schematic for THz generation. The circular THz emitter array is shown above to miniaturize the device by providing 10 megawatts of seed power to the THz beam.

Project Description

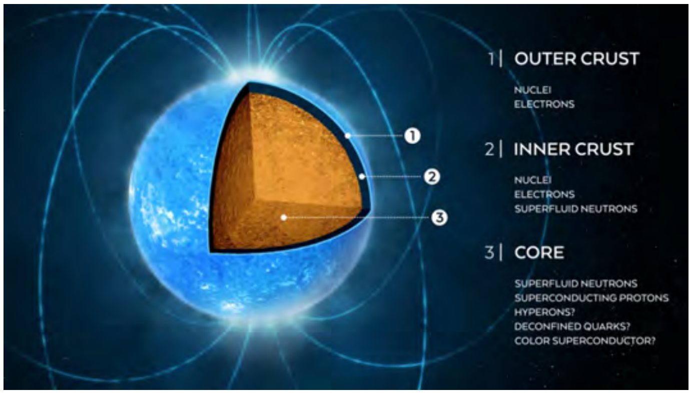
The project addresses several national security challenges: 1. Everyone knows about millimeter-wave security screening at airports (30-300 gigahertz (GHz)). Unlike those mm-wave imaging, Terahertz (THz) imaging (300-3000GHz) can be used anywhere to detect concealed chemical weapons, drugs and improvised explosive devices (IED). Right now, the state-of-the-art THz sources provide too little power for accurate signal detection and imaging. This project aims to address this problem. A free electron laser (FEL) system can provide several tens of watts of THz power that can be used for security imaging, short-range radars and high speed surveillance systems. 2. The project directly studies the physics involved in miniaturization of large FEL systems, thereby addressing the Department of Energy's (DOE's) mission on compact accelerator systems. These compact accelerators can be used for food safety and medical purposes such as cancer detection, destroying cancer cells etc. 3. The study of the seeding method directly relates to the Laboratory's Dynamics Mesoscale Material Science Capability (DMMSC). The seeding method can be generalized to x-ray FEL system if proven successful. This addresses the DOE/National Nuclear Security Administration mission on making compact X-ray sources and detectors.

Technical Outcomes

The technical goal of the project was to determine the feasibility of using Terahertz (THz) seeding for generating high power THz. The team successfully showed through numerical simulation that the seeding helps to miniaturize the overall footprint of the device a within few meters. Also, the team found a suitable space-borne accelerator design that will support the idea of realizing compact, portable High-power THz source. The project successfully studied the technical merit of the design.

The Nuclear Equation of State from Analyses of Merging Neutron Stars

Ingo Tews
20220658ER



Shown is the neutron-star structure from low densities in the crust to high-densities in the core. This project will provide a full microphysical modeling of the equation of state over the full density range with uncertainties and temperature effects. We will combine quantum Monte Carlo calculations, that can describe the structure down to the outer core, with explicit quantum chromodynamics (QCD) modeling that describes the inner core. Image Credit: A. Watts et al., Rev. Mod. Phys. 88, 021001 (2016).

Project Description

The work will involve the heavy use of supercomputers for large-scale calculations of dense nucleonic matter present in neutron stars. To date, there are no theoretical models for this matter that account for all known effects and all theoretical uncertainties. We will be the first ones to provide such modeling. The matter in neutron stars is denser and more neutron-rich than any matter that can be attained in laboratories and its study complements experiments as done by, e.g., the Facility for Rare Isotope Beams. Advancing our ability to calculate the properties of matter will allow us to advance the state of the art in predicting nuclear physics in regimes where experiments are difficult or impossible, like reactions on unstable nuclei. Our results will be important for comparisons with nuclear experiments performed by the Department of Energy but also for gravitational wave detectors like the Laser Interferometer Gravitational-wave Observatory (LIGO) and Virgo.

Technical Outcomes

The project combined numerical quantum Monte Carlo calculations valid at densities up to twice the nuclear saturation density with different high-density models for the neutron star (NS) interior. In these environments, understanding of the equation of state (EOS) is uncertain and exotic phases of matter are expected to appear whose properties are not well understood. Data-analysis tools were developed to compare EOS models with astrophysical observations of NS and nuclear experiments performed at heavy-ion colliders.

Publications

Journal Articles

Afle, C., P. R. Miles, S. Caino-Lores, C. D. Capano, I. Tews, K. Vahi, D. A. Brown, E. Deelman and M. Taufer. Reproducing the results for NICER observation of PSR J0030+0451. Submitted to *Computing in Science & Engineering*. (LA-UR-22-29359)

Alford, M. G., L. Brodie, A. Haber and I. Tews. Relativistic mean-field theories for neutron-star physics based on chiral effective field theory. 2022. *Physical Review C*. **106** (5): 055804. (LA-UR-22-23972 DOI: 10.1103/PhysRevC.106.055804)

*Huth, S., P. T. H. Pang, I. Tews, T. Dietrich, A. Le Fevre, A. Schwenk, W. Trautmann, K. Agarwal, M. Bulla, M. W. Coughlin and C. Van den Broeck. Constraining neutron-star matter with microscopic and macroscopic collisions. 2022. *Nature*. **606** (7913): 276-280. (LA-UR-21-22072 DOI: 10.1038/s41586-022-04750-w)

Pang, P. T., T. Dietrich, M. W. Coughlin, M. Bulla, I. Tews and C. Van Den Broeck. NMMA: A nuclear-physics and multi-messenger astrophysics framework to analyse binary neutron star mergers. Submitted to *Nature Scientific Reports*. (LA-UR-22-23872)

Rose, H., N. Kunert, T. Dietrich, P. T. H. Pang, R. Smith, C. Van den Broeck, S. Gandolfi and I. Tews. Revealing the strength of three-nucleon interactions with the Einstein Telescope. Submitted to *Physical Review Letters*. (LA-UR-22-21458)

Schatz, H., A. D. Becerril Reyes, A. Best, E. F. Brown, K. Chatziioannou, K. A. Chipps, C. M. Deibel, R. Ezzeddine, D. K. Galloway, C. Hansen, F. Herwig, A. Ji, M. Lugaro, Z. Meisel, D. Norman, J. Read, L. F. Roberts, A. Spyrou, I. Tews, F. X. Timmes, C. Travaglio, N. Vassh, A. J. Couture, C. L. Fryer, A. E. Lovell, M. R. Mumpower and T. M. Sprouse. Horizons: nuclear astrophysics in the 2020s and beyond. 2022. *Journal of Physics G: Nuclear and Particle Physics*. **49** (11): 110502. (LA-UR-22-23997 DOI: 10.1088/1361-6471/ac8890)

Somasundaram, R., I. Tews and J. Margueron. Importance of Perturbative QCD Calculations for Studies of Neutron Stars. Submitted to *Physical Review Letters*. (LA-UR-22-22575)

Ujevic, M., H. Gieg, I. Tews, F. Schianchi, S. V. Chaurasia and T. Dietrich. Back and Forth: A Reverse Phase Transitions in Numerical Relativity Simulations. Submitted to *Physical Review D*. (LA-UR-22-31740)

Presentation Slides

King, B. L., I. Tews and S. De. Investigating Systematic Biases when Inferring the Nuclear Equation of State from Astrophysical Data. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-01. (LA-UR-22-28342)

Paris, M. W. and E. Grohs. w20_qBURST Results. . (LA-UR-22-26030)

Tews, I., B. L. King and S. De. Investigating Systematic Biases when Inferring the Nuclear Equation of State from Astrophysical Data. . (LA-UR-22-28346)

Tews, I. and D. Lonardoni. The nuclear equation of state at neutron-proton asymmetries (w21_eosafdmc). . (LA-UR-23-23206)

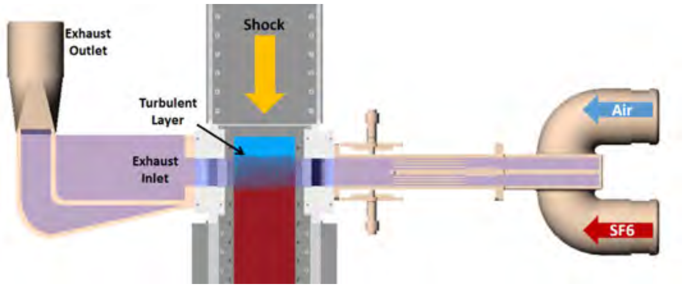
Posters

Tews, I., B. L. King and S. De. Investigating Systematic Biases when Inferring Nuclear Equation of State from Astrophysical Data. . (LA-UR-22-27596)

**Peer-reviewed*

Shocked Variable-Density Turbulence

Tiffany Desjardins
20210601ECR



Shocks interacting with a turbulent layer are common in astrophysics and inertial confinement fusion layers, but are difficult to study in a laboratory setting. On the Vertical Shock Tube the team is able to cross-flow two different density gases; by adjusting the inflow conditions the team can create a mixing and turbulent layer and use high speed diagnostics to capture the dynamics as a shock crosses and interacts with that layer. Understanding how shocks affect turbulence will enable the project team to improve current and future models and simulations developed by LANL.

Project Description

Without underground testing, we rely on simulations to validate the integrity of the nation's stockpile. Los Alamos has been developing some of the most advanced simulation codes in order to model the complex physics involved. To both improve and validate these codes, we need to develop simplified experiments that allow us to target a specific piece of physics. This project aims to study one such piece: the interaction of a shock wave with variable-density turbulence, i.e., two fluids with large density differences mixing together. This interaction occurs in supernova and inertial confinement fusion implosions. Despite years of study, we still have difficulty in accurately predicting the outcome of such systems. By studying the effects a shock has on variable-density turbulence, we can develop a physical understanding of this complex interaction. The results will be used to develop simplified models that must be integrated into our existing simulation and computing codes. Improvement of these codes will aid in the assurance of our nation's existing and future stockpile.

Publications

Presentation Slides

Desjardins, T. Shocked Variable-Density Turbulence. Presented at *IWPCTM*, Atlanta, Georgia, United States, 2022-07-17 - 2022-07-22. (LA-UR-22-26878)

Desjardins, T., J. J. Charonko and A. A. Martinez. Studying the Interaction of Shocks and Turbulence in a Variable-Density Experiment. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Fluid Dynamics (DFD)*, Indianapolis, Indiana, United States, 2022-11-20 - 2022-11-22. (LA-UR-22-32372)

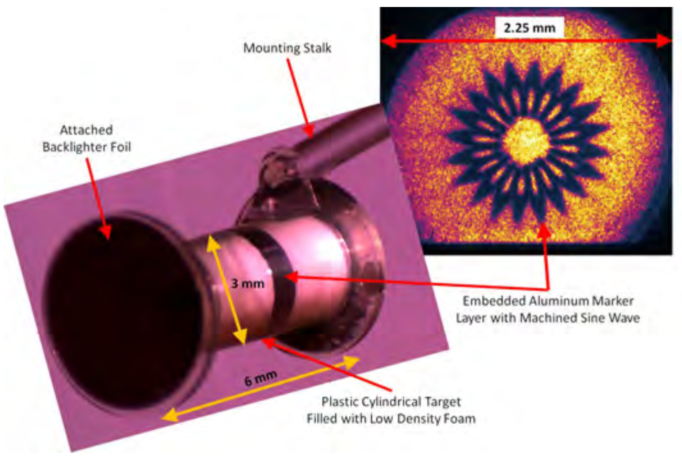
Posters

Desjardins, T., J. J. Charonko and S. L. Pellone. (U) Shocked Studies of Gaseous Interfaces. Presented at *Nuclear Explosives Design Physics Conference (NEDPC)*, Livermore, California, United States, 2022-11-07 - 2022-09-08. (LA-CP-22-20752)

**Peer-reviewed*

Diagnosing Plasma Viscosity in Compressible High-Energy-Density Systems

Joshua Sauppe
20210659ECR



Los Alamos scientists use cylindrical implosions to directly diagnose hydrodynamic instability growth in a convergent geometry, enabling tests of detailed physics models in a high-energy-density system. These experiments, fielded at the OMEGA laser facility and the National Ignition Facility, directly drive the cylinder with laser light, and radiographic images provide high quality data during the implosion. This research uses radiation-hydrodynamics simulations to push the existing experimental platform to conditions in which the plasma viscosity is important to instability growth, and this is expected to enable the first direct measurements of viscosity in this regime.

Project Description

Stockpile stewardship requires a thorough understanding of how matter behaves under extreme conditions. This project will focus on improving our understanding of the plasma viscosity. In contrast to low-energy-density fluid systems, the viscosity in a weakly coupled plasma rises rapidly as the temperature increases, and viscosity is predicted to provide some stabilization of hydrodynamic instability growth which can occur in imploding systems such as inertial confinement fusion (ICF) targets. Because these instabilities can contribute to material mixing in ICF implosions, accurately capturing this growth is essential to improving the predictive capability of our radiation-hydrodynamics codes. The primary goal of this research is to develop a cylindrical implosion target design that can be used to directly measure the stabilizing effects of plasma viscosity on such instability growth. The research is expected to result in several designs that could be fielded on laser facilities in the near future, providing very useful validation data for our models in these high-energy-density regimes.

Publications

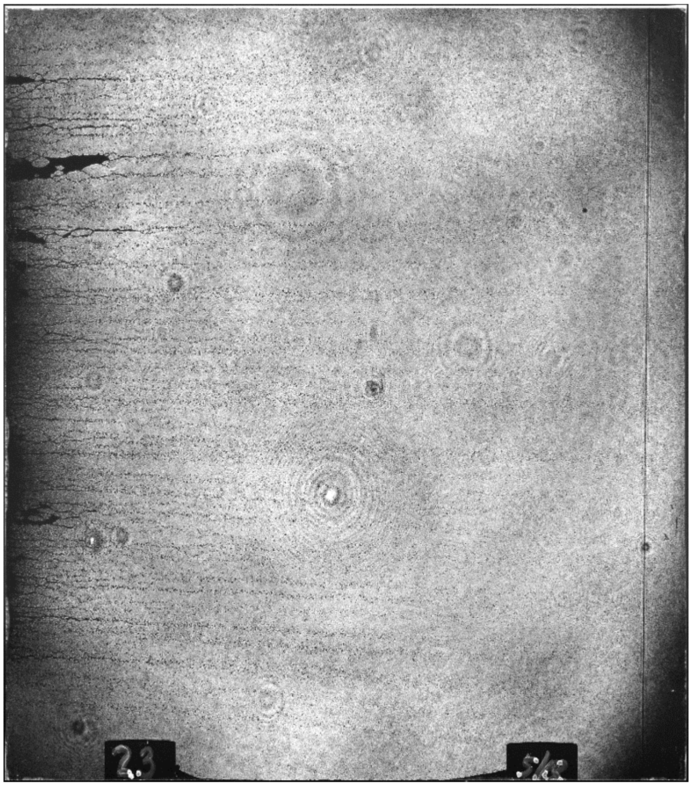
Reports

Keenan, B. Verification study of xRAGE's multi-ion viscosity model. Unpublished report. (LA-UR-22-27763)

**Peer-reviewed*

MEGAgram (Measurements of Ejecta in GAs): Digital Holography for Ejecta in Extreme Conditions

Dana Duke
20210695ECR



A hologram of ejecta particles recorded on film. The ejecta from shocked tin metal travels from left to right in this snapshot of shocked material breakup due to Richtmyer-Meshkov instabilities. This work will improve ejecta measurements by recording ejecta images with a digital high-speed camera.

Project Description

As an explosively driven shock wave impacts machined grooves in a metal surface, it ejects a cloud of the material, known as "ejecta". The physics and behavior of ejecta is important for national security interests, however the experiments are challenging. Scientists must measure microscopic particles propelled by high-explosives at supersonic speeds through high temperature gas. MEGAgram (Measurements of Ejecta in GAs Holograms) will produce the first ever multi-frame digital holographic rendering of micron-scale ejecta in these national security-relevant and previously inaccessible environments. Utilizing cutting-edge laser and digital imaging technology, MEGAgram's goal is to provide scientists a multi-frame, 3-Dimensional look into evolving ejecta behavior as it moves through gas. The successful MEGAgram experiments will enable new discoveries about ejecta physics and provide new data. This mission-focused capability will help the United States Department of Energy/National Nuclear Security Administration gain a critical advantage in modeling complex, dynamic systems.

Publications

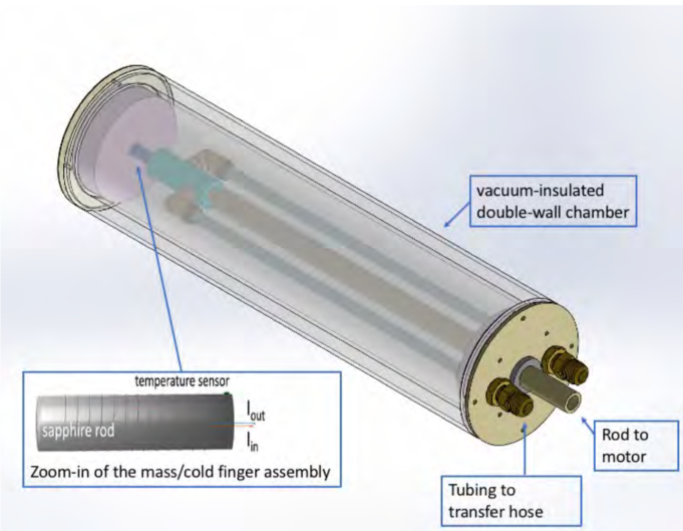
Journal Articles

Guildenbecher, D. R., A. McMaster, A. C. Corredor, R. M. Malone, J. Mance, E. D. Rudziensky, D. Sorenson, J. Danielson and D. L. Duke. Ultraviolet Digital Holographic Microscopy (DHM) of micron-scale particles from shocked Sn ejecta. Submitted to *Journal of Applied Physics*. (LA-UR-22-32623)

**Peer-reviewed*

Searches for Exotic Spin-Dependent Interactions using a Spin-Exchange Relaxation-Free Magnetometer and a Rare-Earth Iron Garnet Mass

Pinghan Chu
20210750ECR



The goal of this project is to measure the exotic spin-spin-velocity-dependent interactions using the quantum sensing spin exchange relaxation-free (SERF) magnetometer with polarized dysprosium-iron garnet (DyIG) mass. The magnetic effect of the mass can be minimized by keeping it at the critical temperature 240 K. The tubing is connected to the hoses to transfer cold liquid from the Dewar to the mass/cold finger assembly and this vacuum-insulated double-wall chamber is designed to reduce the thermal fluctuation. The success of the project will be of interest to quantum sensing in precision measurement and opportunities in nuclear and particle physics, one of the LANL/DOE pillar missions.

Project Description

This project will utilize world-leading expertise in Los Alamos in development and application of spin-exchange relaxation-free magnetometers, one of the most sensitive quantum magnetic-field sensors. While exploring exotic spin-dependent interactions between two particles, mediated by new bosonic particles, has been of keen interest in solving the most profound modern physics puzzles, such as the matter-antimatter asymmetry of the Universe and the nature of dark matter, the high energy physics (HEP) and nuclear physics communities have also developed growing interest in quantum sensing in precision measurement and discovery of new physics. Recently, Department of Energy (DOE) has announced a program in HEP-Quantum Information Science (QIS), "Quantum Information Science Enabled Discovery (QuantISED)", aligned with the "Science First" driver for the national QIS program. This pioneering idea using quantum sensors with the polarized mass of zero magnetization provides a promising method for fundamental searches in nuclear physics, particle physics, and astrophysics.

Publications

Journal Articles

Chu, P. -., N. Ristoff, J. Smits, N. Jackson, Y. J. Kim, I. Savukov and V. M. Acosta. Proposal for the search for new spin interactions at the micrometer scale using diamond quantum sensors. 2022. *Physical Review Research*. **4** (2): 023162. (LA-UR-22-20703 DOI: 10.1103/PhysRevResearch.4.023162)

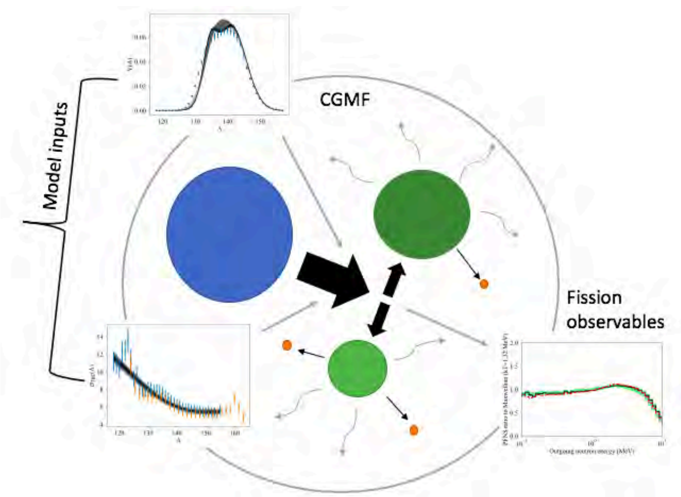
Presentation Slides

Chu, P. Search for New Physics With atomS. Presented at *OSE Seminar*, Albuquerque, New Mexico, United States, 2022-03-31 - 2022-03-31. (LA-UR-22-22949)

**Peer-reviewed*

Global Optimization of Correlated Fission Observables with Quantified Uncertainties

Amy Lovell
20220532ECR



CGMF (Cascading Gamma Multiplicity for Fission) is ideally suited to model complex correlations among prompt fission observables, by consistently modeling fission from the formation of the compound nucleus (blue) to the splitting into two fragments (green) and emission of neutrons (orange) and gamma rays (gray curved lines). Including uncertainties on the input parameters (gray bands) can be propagated through CGMF to provide robust uncertainties on fission observables (green band). This optimization framework will improve CGMF for applications and will be generalizable beyond fission modeling.

Project Description

Fission modeling is important for a variety of applications including nonproliferation, stockpile stewardship, energy, and our fundamental understanding of this complex process. This project will provide the capability to consistently and simultaneously optimize model inputs over all prompt (short-time) neutron and gamma-ray fission observables, with an emphasis on robust theoretical uncertainty quantification. We will optimize the fission model inputs, not only to the observable that is most sensitive, but to all observables simultaneously, allowing us to explore the full input space for the first time. Consistent modeling will improve nuclear data evaluations that are vital input for nuclear applications, including transport calculations that are crucial for modeling reactors and weapons applications. In particular, the robust optimization and uncertainty quantification will target the energy spectrum of the outgoing fission neutrons which is notoriously difficult to model. An improvement in this energy spectrum can have significant modeling impacts in the above applications. Lastly, the framework that will be developed through this project will be widely applicable to other nuclear physics codes, leading to improved optimization and uncertainty quantification across the nuclear theory community.

Publications

Journal Articles

Hebborn, C., F. M. Nunes and A. E. Lovell. New perspectives on spectroscopic factor quenching from reactions. Submitted to *Physical Review Letters*. (LA-UR-23-21722)

Hebborn, C., T. R. Whitehead, A. E. Lovell and F. M. Nunes. Quantifying uncertainties due to optical potentials in one-neutron knockout reactions. Submitted to *Physical Review C*. (LA-UR-22-32049)

Reports

Lovell, A. E. CGMF Data Comparison. Unpublished report. (LA-UR-22-29191)

Presentation Slides

Beyer, K. A., A. E. Lovell, P. Cole and B. C. Kiedrowski. Extending optical models to the fission fragment region. . (LA-UR-22-32971)

Lovell, A. E. Uncertainty Quantification in Reaction Theory. Presented at *Low Energy Community Meeting*, Online, New Mexico, United States, 2022-08-08 - 2022-08-10. (LA-UR-22-28156)

Lovell, A. E. Uncertainty quantification for fission modeling. . (LA-UR-22-32371)

Lovell, A. E. Exploring Fission Fragment Initial Conditions with Robust Uncertainty Quantification. . (LA-UR-23-23154)

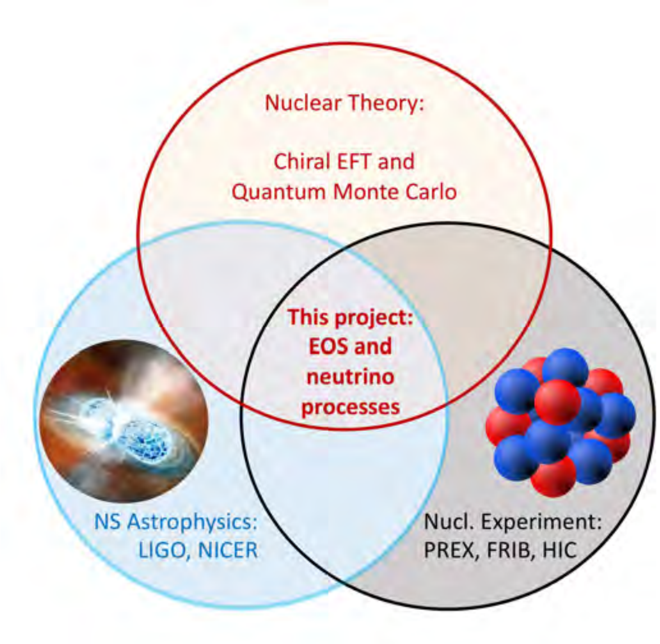
Posters

Lovell, A. E. Uncertainty quantification for optical model parameters and cross sections. . (LA-UR-23-22698)

**Peer-reviewed*

Precision Studies of Nuclear Matter and Neutrino Interactions for Multimessenger Astrophysics

Ingo Tews
20220541ECR



The research project is at the forefront of new discoveries in science, at the intersection of nuclear theory, experiment, and astrophysics. It will combine state-of-the-art calculations performed at LANL, astrophysical data from NASA and gravitational-wave observatories, e.g., LIGO, experimental results from facilities like the Facility for Rare Isotope Beams, and the Thomas Jefferson National Accelerator Facility, to pin down the properties of dense nuclear matter and their neutrino interactions with high precision.

Project Description

This project will involve the heavy use of supercomputers for large-scale calculations of dense nucleonic matter present in neutron stars and neutrino scattering with this matter. In particular, this project will considerably improve theoretical uncertainties in the prediction of these systems by advancing theoretical models describing the interactions in these systems. The matter in neutron stars is denser and more neutron-rich than any matter that can be attained in laboratories and its study complements experiments as done by, e.g., the Facility for Rare Isotope Beams. Advancing our ability to calculate the properties of dense matter will allow us to advance the state of the art in predicting nuclear physics in regimes where experiments are difficult or impossible, like reactions on unstable nuclei. The results of this project will be important for the analysis of data collected by gravitational wave detectors like the Laser Interferometer Gravitational-wave Observatory (LIGO), the National Aeronautics and Space Administration's (NASA) Neutron-Star Interior Composition Explorer mission, as well as nuclear experiments performed by the Department of Energy.

Publications

Journal Articles

Afle, C., P. R. Miles, S. Caino-Lores, C. D. Capano, I. Tews, K. Vahi, D. A. Brown, E. Deelman and M. Taufer. Reproducing the results for NICER observation of PSR J0030+0451. Submitted to *Computing in Science & Engineering*. (LA-UR-22-29359)

Chamseddine, M., J. Margueron, G. Chanfray, H. Hansen and R. Somasundaram. Relativistic Hartree-Fock Chiral Lagrangians with confinement, nucleon finite size and short-range effects. Submitted to *European Journal of Physics*. (LA-UR-23-23392)

Kunert, N., S. Antier, V. Nedora, M. Bulla, P. T. Pang, M. W. Coughlin, W. Kiendrebeogo, I. Tews, M. Pilloix, J. Barnes and T. Dietrich. Model selection for GRB 211211A through multi-wavelength analyses. Submitted to *Astrophysical Journal*. (LA-UR-22-32364)

Rose, H., N. Kunert, T. Dietrich, P. T. H. Pang, R. Smith, C. Van den Broeck, S. Gandolfi and I. Tews. Revealing the strength of three-nucleon interactions with the Einstein Telescope. Submitted to *Physical Review Letters*. (LA-UR-22-21458)

Reports

Sorensen, A., I. Tews, S. Gandolfi, W. Newton and C. Drischler. Dense Nuclear Matter Equation of State from Heavy-Ion Collisions. Unpublished report. (LA-UR-23-20514)

Presentation Slides

Tews, I. Nuclear-Matter Theory: Introduction to chiral effective field theory. Presented at *ACFI workshop "The Future of Neutron Rich Matter: From Neutron Skins to Neutron Stars"*, Amherst, Massachusetts, United States, 2022-10-13 - 2022-10-13. (LA-UR-22-30748)

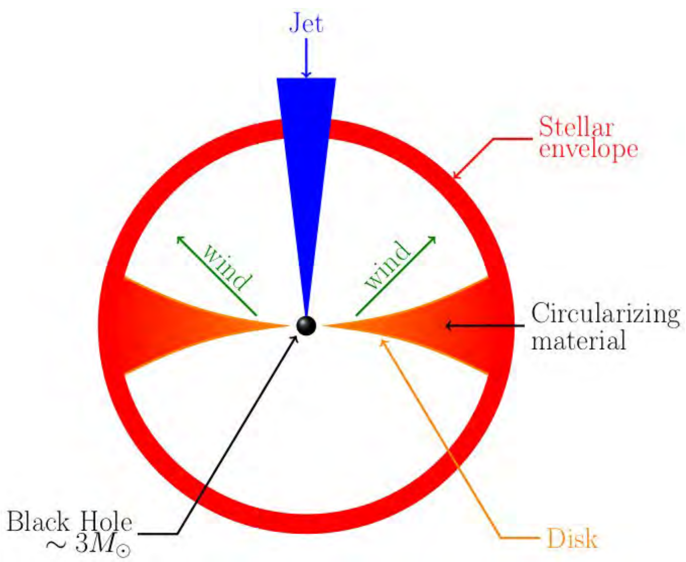
Tews, I. Constraining the nuclear EOS with theory, observations, and experiment. Presented at *INT Workshop 22-84W: 'Dense Nuclear Matter Equation of State from Heavy-Ion Collisions'*, virtual, Washington, United States, 2022-12-05 - 2022-12-09. (LA-UR-22-32682)

Tews, I. From Nuclei to Neutron Stars: Constraining the nuclear EOS with Theory, Experiment, and Multi-messenger Observations. . (LA-UR-23-21296)

**Peer-reviewed*

High-Resolution, Full-Physics Modeling of Failed Supernovae: Are Collapsars a Source of Heavy Elements in the Universe?

Jonah Miller
20220564ECR



When a massive, rapidly rotating star runs out of nuclear fuel, it can form a collapsar. The core of the star becomes a black hole. The stellar envelope (red) forms a disk (orange) that orbits and falls into the black hole. This powers a jet of material moving near the speed of light (blue) and a wind of hot, neutron-rich gas (green). The wind and jet may be sites for the fusion of heavy elements. Scientists at Los Alamos National Laboratory are modeling this enigmatic system with state of the art supercomputer simulations. [Image credit: Los Alamos National Laboratory]

Project Description

The heaviest elements in the universe are formed by rapid neutron capture, or r-process nucleosynthesis. These elements play an essential role in living things, so the search for the origins of heavy elements is a search for the origins of life itself. One long considered source of r-process elements is the collapse of a massive, rapidly rotating star. We will perform the highest-fidelity simulations to-date of these complex and enigmatic systems, and determine whether or not they can be a major contributor to measured r-process abundances. The Nuclear Science Advisory Committee long range plan highlights both the origin of heavy elements and the deaths of stars as key science goals. The National Nuclear Security Administration (NNSA) mission requires high-fidelity, multi-scale, multi-physics modeling of systems important to the Nation. As we reach the end of Moore's law, computing hardware becomes ever-more-specialized. The former need and the latter trend are what motivated the development of the Phoebus code. We will stress test Phoebus in a new context, and are well positioned to bring lessons learned into the weapons program.

Publications

Journal Articles

Barker, B. L., E. O'Connor and S. Couch. Inferring Type II-P Supernova Progenitor Masses from Plateau Luminosities. 2023. *The Astrophysical Journal Letters*. **944** (1): L2. (LA-UR-22-31879 DOI: 10.3847/2041-8213/acb052)

Curtis, S., J. M. Miller, C. Frohlich, T. M. Sprouse, N. M. Ronning and M. R. Mumpower. Nucleosynthesis in Outflows from Black Hole-Neutron Star Merger Disks With Full GR$\u $RMHD. Submitted to *Astrophysical Journal Letters*. (LA-UR-22-32395)

Wolfe, N. E., C. Frohlich, J. M. Miller, A. Torres-Forne and P. Cerda-Duran. Gravitational Wave Eigenfrequencies from Neutrino-Driven Core-Collapse Supernovae. Submitted to *Astrophysical Journal*. (LA-UR-23-21532)

Presentation Slides

Miller, J. M. Nuclear Astrophysics and Astrophysical Transients. . (LA-UR-22-32347)

Miller, J. M. Compact Object Astrophysics At Scale: Experiences on GPUs and Chicoma. . (LA-UR-23-22909)

Miller, J. M. The Aftermath of a Black Hole Eating a Neutron Star. . (LA-UR-23-23315)

Miller, J. M., K. A. Lund and G. C. McLaughlin. Neutrino Transport and Effects on Observables in Compact Binary Mergers. Presented at *43rd International School of Nuclear Physics*, Erice, Italy, 2022-09-16 - 2022-09-22. (LA-UR-22-29453)

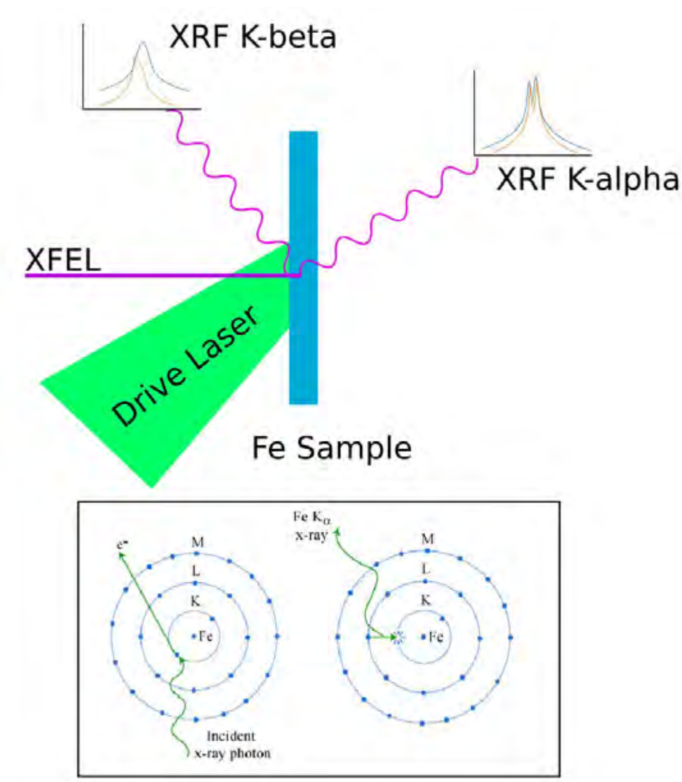
Miller, J. M., S. Curtis, K. Lund and G. McLaughlin. Post-Merger Disks with Full Neutrino Physics. Presented at *Remnants of Neutron Star Mergers*, Darmstadt, Germany, 2022-10-17 - 2022-10-20. (LA-UR-22-30769)

Miller, J. M., S. Curtis, M. V. Urrutia Hurtado, K. A. Lund and B. L. Barker. Impact of Neutrinos in Post-Merger Accretion FLows. Presented at *Kilonova: Multimessenger and Multiphysics*, Bad Honnef, Germany, 2022-11-28 - 2022-12-01. (LA-UR-22-32338)

**Peer-reviewed*

Diagnosis of Low Temperature Compressed Systems

Pawel Kozlowski
20220596ECR



The proposed x-ray fluorescence spectroscopy capability will enable direct measurements of temperature and ionization of shock compressed mid-Z to high-Z elements (elements with mid-to high atomic numbers) at x-ray free electron laser facilities. This will provide high-resolution insights into the warm dense matter state.

Project Description

Experiments on warm dense matter systems, which are generated when materials are subjected to high pressure conditions, are critical to our understanding of material dynamics, and electronic structure in extreme conditions. Warm dense matter experiments are typically conducted at the Department of Energy's various laser facilities (e.g. The National Ignition Facility, and Omega-60). At present, most diagnostics used at these facilities can only probe these states indirectly, and those few x-ray diagnostics which can probe these states directly often suffer from noise and interpretation issues. By leveraging new x-ray laser sources, such as the Linac Coherent Light Source, we will develop a novel x-ray fluorescence spectroscopy diagnostic for directly measuring temperature and ionization of these exotic states of matter with high fidelity. These high resolution measurements will then be used to validate and further develop our capacity to simulate atomic kinetics in these warm dense matter states. This diagnostic platform can then be readily extended to the study of materials composed of elements from the middle and bottom portions of the periodic table of elements, when these materials are subjected to extreme pressure conditions.

Publications

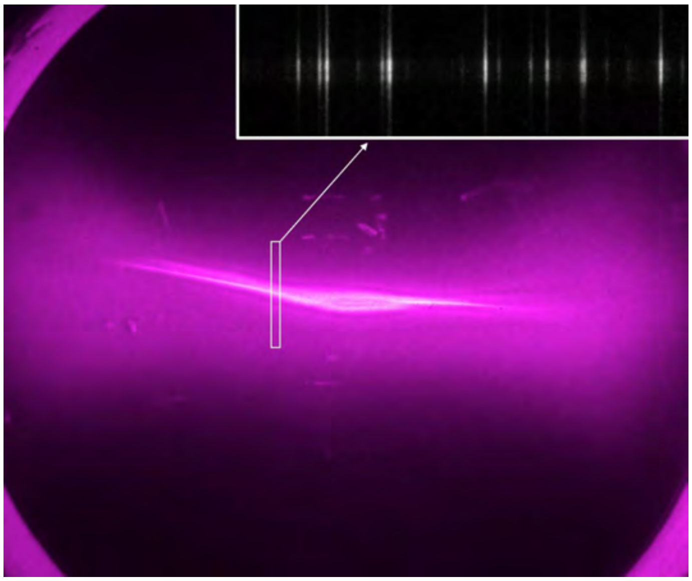
Reports

Kozlowski, P. M., M. J. Macdonald, T. Morrow, S. B. Hansen, A. J. Neukirch, J. P. Colgan and H. J. Lee. Measurement of highly-resolved shifts and splits in x-ray fluorescence lines of warm dense iron. Unpublished report. (LA-UR-22-22892)

**Peer-reviewed*

Resolving Transport Processes in Multispecies Plasma Shock Waves

Samuel Langendorf
20200564ECR



Collisional plasma shocks involving multiple ion species can facilitate species transport and mixing in high-energy density experiments, and there does not presently exist a detailed experimental understanding of their structure. These shocks can be created by the collision of supersonic multispecies plasma jets at the Plasma Liner Experiment (PLX) at LANL, and interrogated by spatially resolved diagnostics such as imaging emission spectroscopy, as pictured. These studies improve the basic understanding of these phenomena and can be used to validate computational models, towards the development of integrated modeling capability.

Project Description

This project seeks to improve the physics basis and predictive capability of Department of Energy (DOE) advanced computer codes. The project seeks to do this by obtaining detailed measurement of a plasma-shock-driven mixing process in a laboratory experiment, using novel detectors enabled by a new type of rotatable mirror array found in modern video projectors. Results are also of basic scientific interest in plasma science and astrophysics.

Technical Outcomes

This project was successful in its overall goal of multi-ion-species plasma shock characterization by way of an extended data-gathering campaign, revealing features of interest including species differential diffusion and ion temperature separation.

Publications

Journal Articles

Chu, F., A. LaJoie, B. Keenan, L. Webster, S. Langendorf and M. Gilmore. Ion Diffusion Velocity Measurements in a Multi-Ion-Species Plasma Shock. Submitted to *Physical Review Letters*. (LA-UR-22-23468)

Presentation Slides

Chu, F. Experimental Measurements of Ion Diffusion Coefficients and Heating in a Multi-Ion-Species Plasma Shock. Presented at *Plasma Physics Seminar at University of California, Irvine*, Irvine, California, United States, 2023-02-28 - 2023-02-28. (LA-UR-23-21890)

Keenan, B., S. Langendorf, F. Chu, A. L. LaJoie and W. Taitano. Multi-Ion Plasma Shock Formation From Colliding Supersonic Jets on the PLX. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30932)

LaJoie, A., F. Chu, L. Webster, S. Langendorf and M. Gilmore. Overview of Present and Planned Diagnostics of the Plasma Liner Experiment (PLX). Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30837)

Posters

Keenan, B., S. Langendorf, F. Chu, A. L. LaJoie and W. Taitano. Multi-Ion Plasma Shock Formation From Colliding Supersonic Jets on the PLX. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30886)

LaJoie, A., F. Chu, L. Webster, S. Langendorf and M. Gilmore. Overview of Present and Planned Diagnostics of the Plasma Liner Experiment (PLX). Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30823)

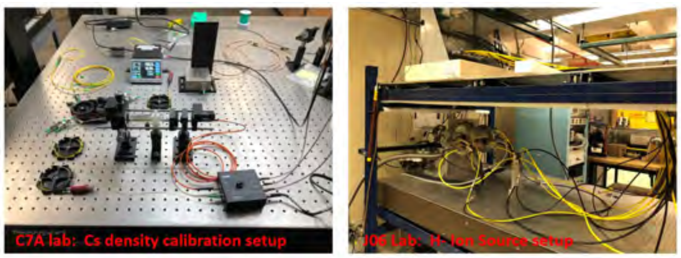
**Peer-reviewed*

Nuclear and Particle Futures

Early Career Research
Final Report

Exploring Inside the Los Alamos Neutron Science Center (LANSCE) Hydrogen- Ion Source with Laser Absorption Techniques

David Kleinjan
20200570ECR



This project aims to use optical laser techniques to see inside the negative hydrogen ion source to improve its functionality for LANSCE mission needs. The figure's left panel demonstrates the C7A setup to test the laser used to measure cesium density. Some highlighted components are the 852 nanometer diode laser (top-center), and the calibrated cesium glass-cell (center). The figure's right pane l demonstrates the J06 setup of the hydrogen (H)-ion source. Some highlighted components are the H- ion source (left-center), water system (top), vacuum system (left & bottom-left), electronics rack (right-center) are shown.

Project Description

The high energy negative hydrogen ion beam used at the Los Alamos Neutron Science Center's (LANSCE) is created with a negative hydrogen ion source. Using optical laser techniques, we can see inside this ion source. The goal is to increase the overall beam output of LANSCE to meet critical national security needs. This project aims to develop a diagnostic tool using these optical laser techniques to improve the stability and output of the negative hydrogen ion source, and thus the performance of LANSCE. This tool not only has the potential to improve LANSCE mission needs, but once developed, could be utilized by other United States accelerator user facilities to improve their respective beam outputs.

Technical Outcomes

This project successfully built the Los Alamos Neutron Science Center's (LANSCE) negative Hydrogen (H-) Ion Source Laser Diagnostic Stand (HLDS), and it has passed all rigorous safety guidelines at Los Alamos. HLDS uses optical absorption techniques to study cesium and H- ion dynamics inside the LANSCE H- Ion source. It has been fully commissioned to study cesium dynamics, and the capability to study H- dynamics is in place.

Publications

Journal Articles

Kleinjan, D. W., G. Rouleau and L. P. Neukirch. Exploring Inside the LANSCE H- Ion Source with Laser Absorption Techniques. Submitted to *AIP Conference Proceedings*. (LA-UR-20-27331)

Kleinjan, D. W., G. Rouleau and L. P. Neukirch. Exploring Cesium and H- Beam Properties Internal to the LANSCE H- Ion Source Using Resonant Absorption Spectroscopy and Cavity Ring Down Spectroscopy. Submitted to *Journal of Instrumentation*. (LA-UR-22-33199)

Presentation Slides

Kleinjan, D. W. LANL & Max Planck IPP Kickoff Discussions. . (LA-UR-20-21378)

Kleinjan, D. W. Exploring Inside the LANSCE H- Ion Source with Laser Absorption Techniques. Presented at *The 7th International Symposium on Negative Ions, Beams and Sources (NIBS'20). VIRTUAL EVENT*, Los Alamos, New Mexico, United States, 2020-09-01 - 2020-09-11. (LA-UR-20-26755)

Kleinjan, D. W., G. Rouleau and L. P. Neukirch. LANL & Max Planck IPP Collaboration Meeting. . (LA-UR-22-26847)

Kleinjan, D. W., G. Rouleau and L. P. Neukirch. Exploring Cesium and H-beam properties internal to the LANSCE H-Ion Source using Resonant Absorption Spectroscopy and Cavity Ring Down Spectroscopy. Presented at *The 8th International Symposium on Negative Ions, Beams and Sources - NIBS2022*, Padova, Italy, 2022-10-02 - 2022-10-07. (LA-UR-22-30048)

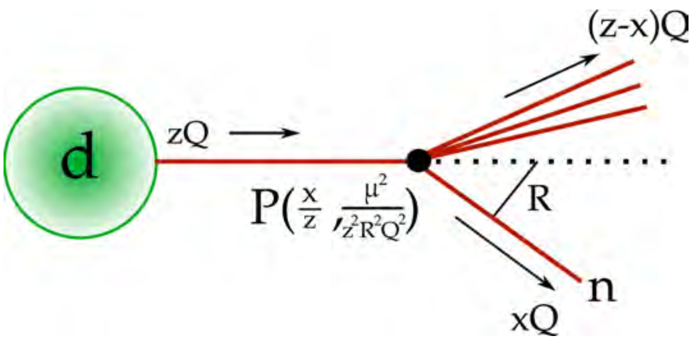
Kleinjan, D. W., L. P. Neukirch and G. Rouleau. LANL & Max Planck IPP 3rd Meeting. . (LA-UR-22-24661)

Kleinjan, D. W. and C. A. Rohde. LANL/Max Planck IPP H-minus Cavity Ringdown Spectroscopy Update. . (LA-UR-23-23479)

**Peer-reviewed*

Quantum Chromodynamics (QCD) Fragmentation Scaling Laws from Space-Time Reciprocity

Duff Neill
20200584ECR



A graphical representation of the fundamental equation that underpins the project. It depicts how the fragmentation spectrum resulting from high-energy nuclear physics collisions evolves with a change in the angular cutoff R. The function d is built from repeated applications of the fundemental splitting process controlled by the kernel P. This kernel is determined by the operators of the underlying quantum field theory that describe the structure of initial states, though the fragmentation process is driven by final state interactions.

Project Description

This work focuses on fundamental science research supported by the Department of Energy (DOE) Office of Science, developing new mathematical techniques for the systematic approximation of non-linear quantum dynamics with many degrees of freedom. This is important for advancing our basic knowledge of the universe, but beyond that, also develops capabilities to tackle and predict some of the most complicated physical processes known to humanity. Such knowledge is paramount in order to therefore prove our capabilities to engineer detectors and experiments that can produce and measure such processes (these having a diverse field of applications), while also showing how one can calculate many other related non-linear strongly interacting quantum systems.

Technical Outcomes

The goal of the project was to calculate the self-similar and fractal properties of quantum chromodynamics (QCD) cascades driven by underlying quantum dynamics. The project successfuly established the resummation in the soft limit of the fragmentation cross-section using relations derived from reciprocity, as was the stated intent. It was hoped that the project would finish the first phenomenological application of these results in proton-electron collisions, but only preliminary results were obtained.

Publications

Journal Articles

Neill, D. A. Local Parton-Hadron Duality Revisited. Submitted to *Journal of High Energy Physics*. (LA-UR-20-27861)

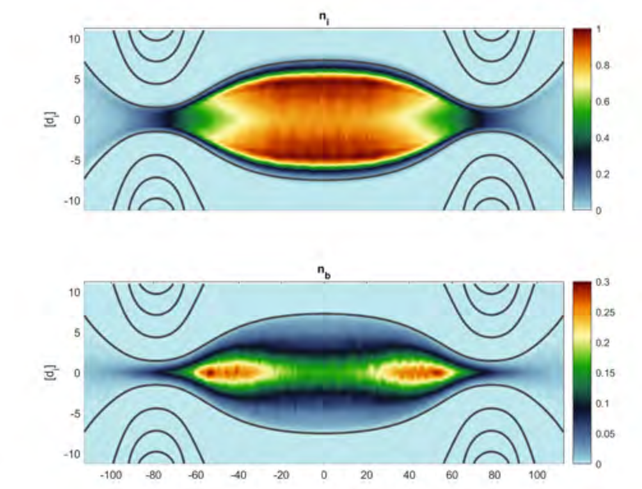
Presentation Slides

Neill, D. A. Fragmentation and Space-Time Reciprocity. . (LA-UR-22-31634)

**Peer-reviewed*

Kinetic Study of a Magnetic-Mirror Wet-Wood-Burner Fusion Neutron Source

Ari Le
20200587ECR



Magnetic mirror fusion devices are being re-visited with modern superconducting coils as promising fusion neutron sources for material and nuclear science studies and, ultimately, as a basis for fusion reactors. The fully kinetic and hybrid vector particle-in-Cell (VPIC) codes are being used to model detailed kinetic transport properties of mirror machines. Kinetic modeling is especially important for understanding fusion performance in devices with both a thermalized background plasma (top) and a fast ions (bottom) injected initially as neutral beams.

Project Description

This project studies the possibility of using a relatively simple and inexpensive magnetic mirror geometry to confine a target plasma of fusion fuel and generate fusion neutrons by bombarding the target plasma with a high-energy beam of additional fusion fuel. Such a fusion neutron source could be used to study material properties under high neutron loads, to diagnose materials, and to prepare rare isotopes for medical and other scientific research. As part of the project, we will develop high-fidelity plasma physics models in a kinetic code that can be used in future studies of fusion in magnetically-confined reactor concepts and high-energy density physics experiments conducted at pulsed power facilities.

Technical Outcomes

A full-device kinetic modeling capability was developed for magnetic mirror confinement schemes that include fast fusion fuel ions. A theory for end losses from the expander region of a magnetic nozzle was verified in detail with particle-in-cell modeling, and three-dimensional stability mirror geometries was studied using a hybrid (kinetic ion/fluid electron) model. High-fidelity simulations explored plasma transport physics relevant to a university mirror experiment under construction through a Department of Energy program.

Publications

*Peer-reviewed

Journal Articles

Le, A. Y., A. J. Stanier, L. Yin, B. A. Wetherton, B. Keenan and B. J. Albright. Hybrid-VPIC: an Open-Source Kinetic/Fluid Hybrid Particle-in-Cell Code. Submitted to *Physics of Plasmas*. (LA-UR-23-21504)

Wetherton, B. A., A. Y. Le, J. Egedal, C. Forest, W. S. Daughton, A. J. Stanier and S. Boldyrev. A drift kinetic model for the expander region of a magnetic mirror. Submitted to *Physics of Plasmas*. (LA-UR-21-20139)

Presentation Slides

Le, A. Y. Example space plasma physics study with Hybrid-VPIC code on Chicoma. . (LA-UR-23-23131)

Le, A. Y., B. A. Wetherton, J. Egedal, C. B. Forest, W. S. Daughton and A. J. Stanier. End Losses from a Magnetic Mirror: Kinetic Simulations and Guiding Center Theory. Presented at *APS Division of Plasma Physics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-28879)

Le, A. Y., L. Yin, A. J. Stanier, B. A. Wetherton, B. Keenan, D. Winske, M. Cowee, F. Guo, Q. Zhang, S. V. Luedtke, W. S. Daughton, B. J. Albright, L. J. Chen, C. Forest, J. Egedal, D. Endrizzi, C. Dong and L. Wang. Hybrid-VPIC Code and Applications. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-17. (LA-UR-22-30756)

Le, A. Y. and B. A. Wetherton. VPIC Mirror Modeling Update. . (LA-UR-21-26113)

Wetherton, B. A. Electron Drift Kinetics in Space and in the Lab. . (LA-UR-22-24878)

Wetherton, B. A., A. Y. Le, A. J. Stanier, J. Egedal and C. B. Forest. Particle-in-cell Modeling of Magnetic Mirror Confinement Devices with VPIC. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30912)

Wetherton, B. A., A. Y. Le, J. Egedal, C. B. Forest, W. S. Daughton, A. J. Stanier and S. Boldyrev. A Drift Kinetic Model for the Expander Region of a Magnetic Mirror. Presented at *WHAM Physics Meeting*, Online, New Mexico, United States, 2021-03-10 - 2021-03-10. (LA-UR-21-22241)

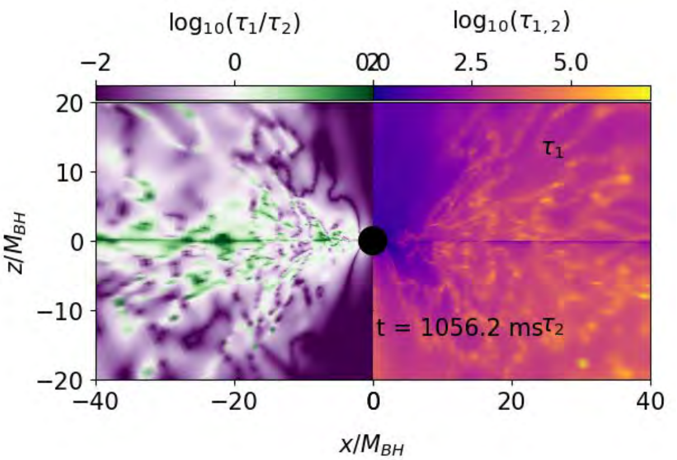
Posters

Le, A. Y. Hybrid-VPIC 3D full-device magnetic mirror simulation preformed on Grizzly. . (LA-UR-22-20816)

Wetherton, B. A., J. Egedal, P. K. Montag, A. Y. Le and W. S. Daughton. A Drift-Kinetic Method for Obtaining Gradients in Plasma Properties From Single-Point Distribution Function Data. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, Remote, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28931)

Towards Data Science Driven Multi-physics Modeling to Probe Neutron Star Mergers

Jonah Miller
20200687PRD2



How violent is the motion of material near a black hole? How much escapes? The LANL code nubhlight can answer these questions. Above is plotted the average time scale of vertical (top right) and horizontal (bottom right) motion of a packet of gas in a disk of material around a black hole. Left panel shows the ratio of the time scales.

Project Description

Modeling the aftermath of neutron star mergers is of critical importance to the scientific community and helps answer fundamental questions such as the nature of matter at high density and the origin of heavy elements in the universe. The previous work at Los Alamos National Lab has not only placed it at the forefront of this effort, but it has also highlighted the many uncertainties that remain uncontrolled in current models. This work will help maintain Los Alamos National Lab's place as a world leader in this field. This project aims to solve a problem that requires a deep understanding of the complex interplay of many processes and an analysis of a high-dimensional dataset. This class of problem is broadly relevant to key laboratory mission areas.

Publications

Journal Articles

*De, S. and D. M. Siegel. Igniting Weak Interactions in Neutron Star Postmerger Accretion Disks. 2021. *The Astrophysical Journal*. **921** (1): 94. (LA-UR-20-28607 DOI: 10.3847/1538-4357/ac110b)

Presentation Slides

De, S. Probing neutron stars with gravitational wave observations. Presented at *Los Alamos Astro Seminar*, Los Alamos, New Mexico, United States, 2021-03-04 - 2021-03-04. (LA-UR-21-22413)

De, S. Project visit LDRD 20200687PRD2. . (LA-UR-21-24500)

De, S. Tidal deformabilities and radii of neutron stars from gravitational-wave observations. Presented at *ECT workshop*, Virtual, Italy, 2021-06-14 - 2021-06-14. (LA-UR-21-25488)

De, S. Probing neutron star mergers with gravity and light. Presented at *Free Mesons Seminar, TIFR Bombay*, Virtual, India, 2021-07-22 - 2021-07-22. (LA-UR-21-27041)

De, S. Parameter estimation for experiments in astrophysics and hydrodynamics: techniques and infrastructures. Presented at *ANSI Seminar*, Los Alamos, New Mexico, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-30094)

De, S. Learning physics from data: techniques for physics-informed inverse analysis of data from experiments and simulations. Presented at *COSIM seminar, LANL*, Los Alamos, New Mexico, United States, 2022-06-01 - 2022-06-01. (LA-UR-22-25148)

De, S. Learning physics from data: techniques and infrastructures for physics-informed inverse analyses. Presented at *T-5 seminar*, Los Alamos, New Mexico, United States, 2022-06-15 - 2022-06-15. (LA-UR-22-25584)

De, S. Detecting and characterizing the science behind signatures in large data from physics experiments: techniques and digital infrastructures. Presented at *EES Science Cafe, LANL*, Los Alamos, New Mexico, United States, 2022-04-08 - 2022-04-08. (LA-UR-22-28835)

De, S. and D. M. Siegel. Igniting weak interactions in neutron star post merger accretion disks. Presented at *American Physical Society April Meeting 2021*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23687)

Smullen, R. A. and S. De. Black Holes, Crashing Galaxies, and Strange New Planets. . (LA-UR-21-25276)

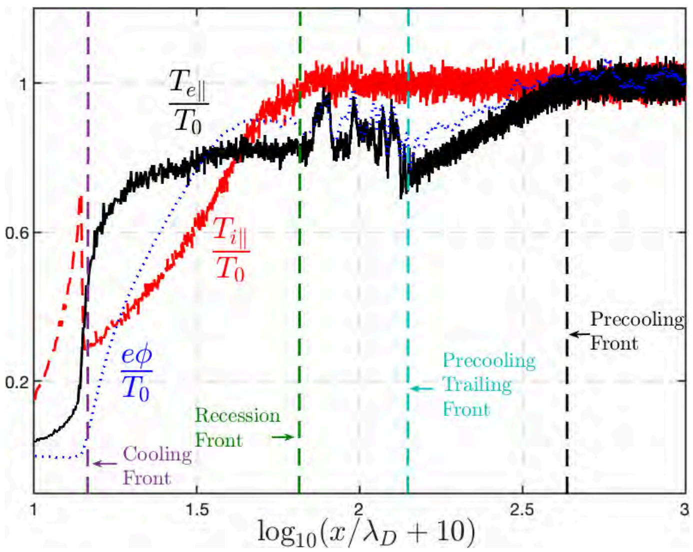
Posters

De, S., M. L. Klasky, O. Korobkin and S. GS. Hydrodynamic parameter estimation using statistical machine learning for dynamic radiography. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-22323)

**Peer-reviewed*

Decipher the Coupled Plasma and Atomic Physics for Reactor Plasma Exhaust

Xianzhu Tang
20200753PRD3



This project integrates the most advanced atomic data produced at Los Alamos National Lab into high-fidelity collisional-radiative models that are then coupled to sophisticated plasma kinetic and fluid solvers. The image provides a schematic view of the cooling flow regime of a nearly collision-less plasma thermal collapse. The thermal collapse comes about in the form of four propagating fronts, all originating from the radiative cooling spot at the left boundary, along the magnetic field lines. The first two are electron fronts with speeds scaling with the electron thermal speed driven by electron thermal conduction in the free-streaming limit. While the last two are ion fronts with nearly local ion sound speeds. Between the ion fronts, the electron thermal conduction is largely reduced from the free-streaming limit to the convective scaling due to the ambipolar transport constraint, which yields a robust cooling flow towards the cooling spot.

Project Description

This project addresses a key scientific and technological challenge in tokamak fusion energy, which if successful, provides a viable emission-free energy source that is a long-term solution to both energy security and climate change. The high-level goals are to understand how detailed atomic physics can impact the plasma exhaust and sustained operation of the steady-state fusion reactor, with the programmatic aim of building the fundamental physics basis for design options and constraints. The approach is to incorporate the state-of-the-art atomic data through a collisional-radiative model into plasma transport modeling, using both the kinetic and fluid approaches. The general scientific problem of how neutrals, plasmas, and radiation interact in a fusion plasma with higher standard deviations from the mean (z-score) impurity is of interest to the inertial confinement fusion problem that is a critical part of the Department of Energy/National Nuclear Security Administration missions. Although the densities are drastically different between the two applications, the fundamental physics approaches and modeling technique are of interests to both applications.

Publications

Journal Articles

Li, J., Y. Zhang and X. Tang. Staged cooling of a fusion-grade plasma in a tokamak thermal quench. Submitted to *Physical Review Letters*. (LA-UR-22-26898)

Li, Y., B. Srinivasan, Y. Zhang and X. Tang. Transport physics dependence of Bohm speed in presheath-sheath transition. 2022. *Physics of Plasmas*. **29** (11): 113509. (LA-UR-22-26588 DOI: 10.1063/5.0110379)

Zhang, Y., J. Li and X. Tang. Cooling flow regime of a plasma thermal quench. Submitted to *Physical Review Letters*. (LA-UR-22-24503)

Zhang, Y., J. Li and X. Tang. Electron heat flux and propagating fronts in plasma thermal quench. Submitted to *Physics of Plasmas*. (LA-UR-22-25987)

Zhang, Y., Y. Li, B. Srinivasan and X. Tang. Resolving the mystery of electron perpendicular temperature spike in the plasma sheath. Submitted to *Physics of Plasmas*. (LA-UR-22-31358)

Zhang, Y. and X. Tang. On the collisional damping of plasma velocity space instabilities. Submitted to *Physical Review Letters*. (LA-UR-22-26897)

Presentation Slides

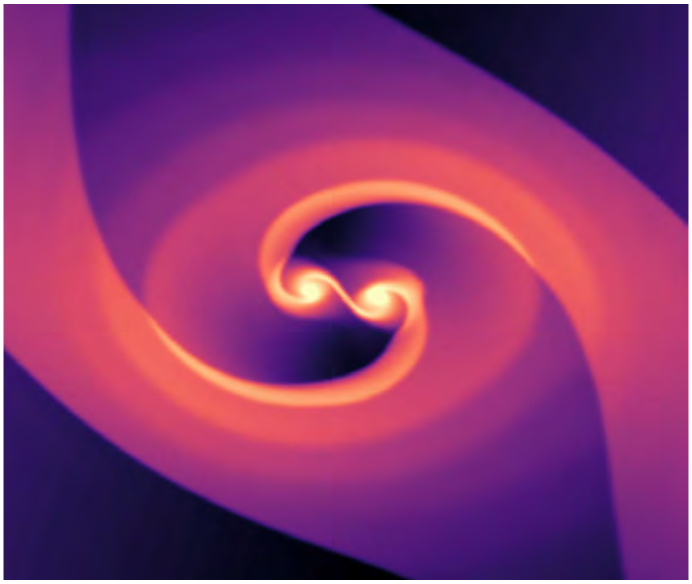
Zhang, Y. Director's postdoc fellow. . (LA-UR-22-21371)

Zhang, Y. Plasma parallel transport physics in a tokamak thermal quench. . (LA-UR-23-23238)

**Peer-reviewed*

The Urge to Merge: The Fate of Binary Black Holes

Hui Li
20200772PRD4



Understanding whether a black hole binary will eventually merge is essential for determining whether they can produce strong gravitational waves or not. Comprehensive multi-dimensional simulations of such binaries, supported by LDRD, reveal a hierarchical structure of disks which govern the angular momentum and mass evolution of the binary, pictured here. [Image credit: Los Alamos National Laboratory]

Project Description

When two black holes get close to each other, whether they will eventually merge or move apart is one of the outstanding questions in modern day astronomy. If they merge, they can produce gravitational waves (GW) signals seen currently by the Laser Interferometer Gravitational-Wave Observatory (LIGO) (for stellar mass black hole binaries), and possibly by Laser Interferometer Space Antenna (LISA (for supermassive black hole binaries)) in the future. The proposed work will produce comprehensive simulations of these sources and develop new tools for high performance computing. It will contribute to the Unites States' LIGO mission and future space-based international LISA mission.

Publications

Journal Articles

F. Calcino, J. P., D. J. Price, H. Garg, B. J. Norfolk, C. Pinte and H. Li. Observational Signatures of Circumbinary Discs I: Theory. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-30251)

*Calcino, J., T. Hilder, D. J. Price, C. Pinte, F. Bollati, G. Lodato and B. J. Norfolk. Mapping the Planetary Wake in HD 163296 with Kinematics. 2022. *The Astrophysical Journal Letters*. **929** (2): L25. (LA-UR-21-31084 DOI: 10.3847/2041-8213/ac64a7)

Garg, H., C. Pinte, I. Hammond, R. Teague, D. Price, J. P. F. Calcino, V. Christiaens and P. Poblete. A kinematic excess in the annular gap and gas depleted cavity in the disc around HD 169142. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-22-31256)

Norfolk, B. J., C. Pinte, J. P. F. Calcino, I. Hammond, N. van der Marel, D. J. Price, S. T. Maddison, V. Christiaens, J. Gonzalez, D. Blakely, G. Rosotti and C. Ginksi. The Origin of the Doppler-flip in HD 100546: a large scale spiral arm generated by an inner binary companion. Submitted to *Astrophysical Journal Letters*. (LA-UR-22-28309)

*Poblete, P. P., N. Cuello, S. Perez, S. Marino, J. Calcino, E. Macias, A. Ribas, A. Zurlo, J. Cuadra, M. Montesinos, S. Zuniga-Fernandez, A. Bayo, C. Pinte, F. Menard and D. J. Price. The protoplanetary disc around HD 169142: circumstellar or circumbinary?. 2022. *Monthly Notices of the Royal Astronomical Society*. **510** (1): 205-215. (LA-UR-21-24101 DOI: 10.1093/mnras/stab3474)

*Verrios, H. J., D. J. Price, C. Pinte, T. Hilder and J. Calcino. Kinematic Evidence for an Embedded Planet in the IM Lupi Disk. 2022. *The Astrophysical Journal Letters*. **934** (1): L11. (LA-UR-21-31387 DOI: 10.3847/2041-8213/ac7f44)

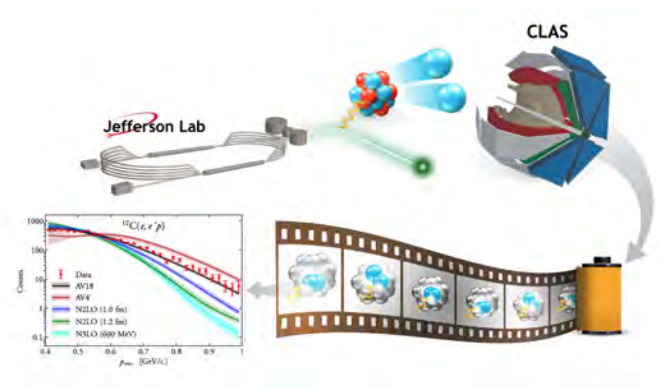
Presentation Slides

F. Calcino, J. P. Eccentric BBHs in AGN Discs: Long and Short Term Evolution. Presented at *AGN Santa Fe*, Santa Fe, New Mexico, United States, 2023-03-22 - 2023-03-24. (LA-UR-23-22640)

**Peer-reviewed*

Short-Range Correlations and Neutrino Interactions in Nuclei

Ronen Weiss
20210763PRD1



High-energy electron beam at the Thomas Jefferson National Accelerator Facility (JLab) is used to knock out short range correlation nucleon pairs from different nuclei. The electron and knock-out protons are measured in the CEBAF Large Acceptance Spectrometer (CLAS) spectrometer (top). Studying many such events, the distribution of closely packed pairs inside the nucleus is assembled and compared to greatest common factor (GCF) theoretical calculations using different models of the nucleon-nucleon interaction (bottom). Correlated triplets and the three-nucleon force can be studied similarly in upcoming JLab experiments, important for the accurate description of nuclear properties. Figure taken from Schmidt et al., Nature volume 578, pages 540–544 (2020).

Project Description

This work will enable us to predict properties of how neutrino interact in large nuclei by including the relevant physics due to short-range correlations.

Publications

Journal Articles

Weiss, R., A. Lovato and R. B. Wiringa. Isospin-symmetry implications for nuclear two-body distributions and short-range correlations. 2022. *Physical Review C*. **106** (5): 054319. (LA-UR-22-23223 DOI: 10.1103/PhysRevC.106.054319)

Weiss, R., P. Soriano, A. Lovato, J. Menendez and R. B. Wiringa. Neutrinoless double-beta decay: combining quantum Monte Carlo and the nuclear shell model with the generalized contact formalism. Submitted to *Physical Review X*. (LA-UR-21-32144)

Weiss, R., S. Beck and N. Barnea. On nuclear short-range correlations and the zero-energy eigenstates of the Schrodinger equation. Submitted to *Physical Review C*. (LA-UR-22-31633)

Weiss, R. and S. Gandolfi. Nuclear three-body short-range correlations in coordinate space. Submitted to *Physical Review Letters*. (LA-UR-22-32748)

Presentation Slides

Weiss, R. Neutrinoless double-beta decay: combining quantum Monte Carlo and the nuclear shell model with the generalized contact formalism. Presented at *INT Program 20r-2b Beyond-the-Standard-Model Physics with Nucleons and Nuclei*, Seattle, Washington, United States, 2022-02-07 - 2022-02-11. (LA-UR-22-20883)

Weiss, R. Confronting SRC data and ab-initio nuclear structure using the GCF. Presented at *Frontiers in Nuclear and Hadronic Physics*, Holderness, New Hampshire, United States, 2022-08-07 - 2022-08-07. (LA-UR-22-27178)

Weiss, R. Generalized Contact Formalism - Recent Advances. Presented at *SRC collaboration meeting*, Boston, Massachusetts, United States, 2022-08-02 - 2022-08-02. (LA-UR-22-27316)

Weiss, R. Generalized Contact Formalism - Three-body correlations. Presented at *SRC collaboration meeting*, Boston, Massachusetts, United States, 2022-08-02 - 2022-08-02. (LA-UR-22-27813)

Weiss, R. Generalized Contact Formalism - Three-body correlations. Presented at *DNP Fall meeting 2022*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-30. (LA-UR-22-31030)

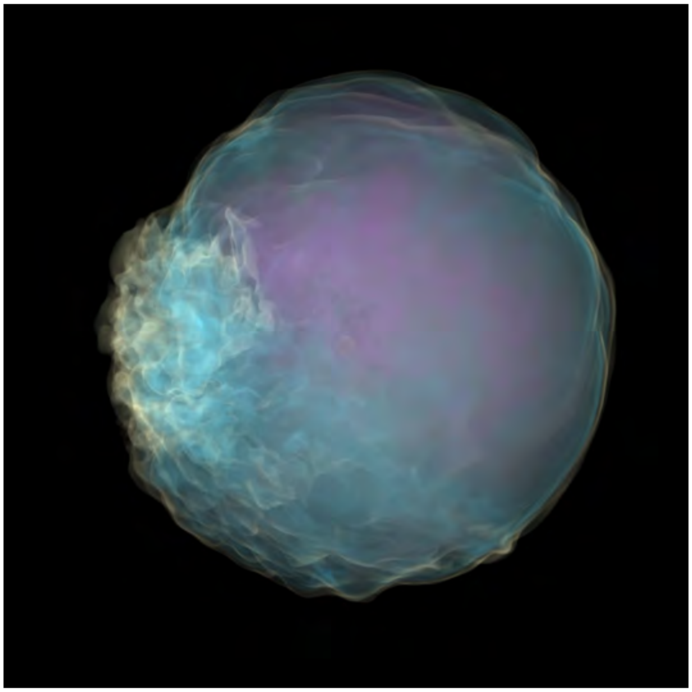
Weiss, R. Applications of the GCF and the study of 3N SRCs. Presented at *4th international workshop on quantitative challenges in short-range correlations and the EMC effect research*, Saclay, France, 2023-01-30 - 2023-01-30. (LA-UR-23-20516)

Weiss, R. Short-range expansion for the nuclear many-body problem. Presented at *FRIB Theory seminar*, East Lansing, Michigan, United States, 2023-02-21 - 2023-02-21. (LA-UR-23-21652)

**Peer-reviewed*

Next Generation Simulations of the Remarkable Deaths of Massive Stars

Carl Fields
20210808PRD1



Volume rendering of the silicon-28 (Si) mass fraction for a three-dimensional hydrodynamic simulation of a massive star less than a second before iron core-collapse. Highlighted are the low (yellow, 0.05), moderate (blue, 0.1), and high (purple, 0.2) concentration of Si. The low concentration regions highlight fresh carbon-12 fuel, blue traces the approximate extent of the convective oxygen-shell, and purple regions follow high concentrations of fresh Si being mixed due to burning. The iron core at this point spans an approximate radius of 2520 kilometers and is shown in gold at the center of the model. Using cutting-edge astrophysics research, we will focus on making predictions for rotating and magnetic core-collapse supernovae, which are the explosive deaths of massive stars.

Project Description

A wide variety of national security challenges require sophisticated computer simulations of phenomena that happen on a wide range of length and time scales. These multi-scale challenges are particularly difficult and developing expertise in this space will be broadly useful for national security applications in the future. To develop this expertise, this work will pursue cutting-edge astrophysics research, studying the explosive deaths of massive stars and making predictions for observations with a variety of facilities.

Publications

Journal Articles

*Fields, C. E. The Three-dimensional Collapse of a Rapidly Rotating 16 M Star. 2022. *The Astrophysical Journal Letters*. **924** (1): L15. (LA-UR-21-31677 DOI: 10.3847/2041-8213/ac460c)

J. Fields, C. E., R. Townsend, F. X. Timmes, M. Zingale and A. Dotter. MESA-Web: A cloud resource for stellar evolution in astronomy curriculum. Submitted to *Astronomy Education Journal*. (LA-UR-22-27884)

*Fields, C. E. and S. M. Couch. Three-dimensional Hydrodynamic Simulations of Convective Nuclear Burning in Massive Stars Near Iron Core Collapse. 2021. *The Astrophysical Journal*. **921** (1): 28. (LA-UR-21-26198 DOI: 10.3847/1538-4357/ac24fb)

Presentation Slides

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-21-24999)

J. Fields, C. E. Assessing the Impact of Uncertainties in Stellar Models. Presented at *INT Program 21-3 - Radionuclides*, SEATTLE, Washington, United States, 2021-10-14 - 2021-10-14. (LA-UR-21-30143)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-21-32036)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-22-20894)

J. Fields, C. E. Next-Generation Simulations of The Remarkable Deaths of Massive Stars. . (LA-UR-22-21110)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-22-21390)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-22-22147)

J. Fields, C. E. THE REMARKABLE DEATH OF A MASSIVE STAR. . (LA-UR-22-23581)

J. Fields, C. E. Next-Generation Simulations of The Remarkable Deaths of Massive Stars. . (LA-UR-22-24718)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. Presented at *Transport in Stellar Interiors*, Isla Vista, California, United States, 2021-11-01 - 2021-11-24. (LA-UR-21-31542)

J. Fields, C. E. Next-Generation Simulations of The Remarkable Deaths of Massive Stars. . (LA-UR-21-30583)

J. Fields, C. E. INTRODUCTION TO PARALLEL PROGRAMMING. . (LA-UR-22-27132)

J. Fields, C. E. INTRODUCTION TO GRAPHICS PROCESSING UNITS. . (LA-UR-22-27446)

J. Fields, C. E. THE NEXT GENERATION OF STELLAR ASTROPHYSICS. . (LA-UR-23-21712)

J. Fields, C. E. w22_stars Turbulent Convection in a 19M\xe2\x8a\x99 Star. . (LA-UR-23-23316)

**Peer-reviewed*

Characterizing Strongly-Coupled Plasmas with Subatomic Particles and Jets

Ivan Vitev
20210914PRD2

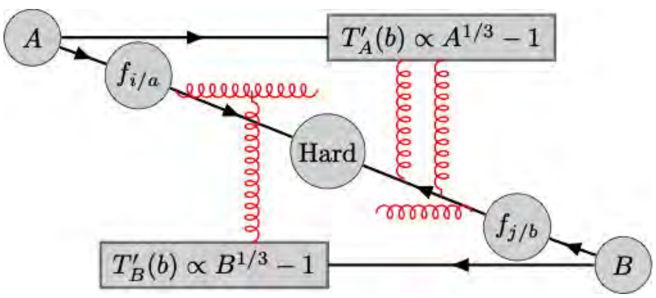


Illustration of the nuclear matter effects that this project will evaluate and include in predictions for light and heavy meson production in collisions of two hadrons or nuclei, A and B. In addition to final-state interactions in the quark-gluon plasma, this work incorporated cold nuclear matter effects that effectively modify the distributions of partons (f) in A and B.

Project Description

One of the main thrusts of modern nuclear physics is to create and characterize extreme states of nuclear matter at the world's highest energy colliders. Such novel state-of-matter, the quark-gluon plasma (QGP), was discovered in experiments at the Relativistic Heavy-Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) and the Large Hadron Collider (LHC) at the European Laboratory for Particle Physics (or Centre Europeenne pour la Recharche Nucleaire-CERN). The quark-gluon plasma is a strongly-interacting "soup" of quarks and gluons, the fundamental building blocks of matter. The major scientific goal of heavy-ion physics is to directly characterize the microscopic degrees-of-freedom of the QGP and probe the dynamical properties of this strongly-coupled and short-lived plasma. Existing RHIC and LHC data on the QGP transport coefficients, however, cannot be quantitatively understood in the framework of a unified theoretical model. The tension between simulations and measurements has prompted detector upgrades at the LHC and new construction, such as the sPHENIX experiment (strongly interacting particles and use of the Pioneering High Energy Nulcear Interaction eXperiment) at RHIC, to further our knowledge of the QGP. To realize the envisioned precision plasma tomography program at RHIC and the LHC, however, concurrent developments in theory and simulation are needed. This project will develop the theory of jets-collimated particle showers-as precision diagnostics of the QGP.

Publications

Journal Articles

Ke, W., M. Xie, H. Zhang and X. Wang. Global constraint on the jet transport coefficient from single hadron, dihadron and $\\gamma$-hadron spectra in high-energy heavy-ion collisions. Submitted to *Physical Review C*. (LA-UR-22-29012)

Ke, W. and I. M. Vitev. Understanding parton evolution in matter from renormalization group analysis. Submitted to *Physical Review Letters*. (LA-UR-23-20730)

Ke, W. and Y. Yin. Does quark-gluon plasma feature an extended hydrodynamic regime?. Submitted to *Physical Review Letters*. (LA-UR-22-27822)

Vitev, I. M. and W. Ke. Searching for QGP droplets with high-pT hadrons and heavy flavor. Submitted to *Journal of High Energy Physics*. (LA-UR-22-23062)

Reports

Ke, W., J. Brewer, L. Yan and Y. Yin. Far-from-equilibrium slow modes and momentum anisotropy in expanding plasma. Unpublished report. (LA-UR-22-32315)

Ke, W., K. Devereaux, W. Fan, K. Lee and I. Moult. Imaging Cold Nuclear Matter with Energy Correlators. Unpublished report. (LA-UR-23-22542)

Ke, W., Z. Yang, Y. He, W. Chen, L. Pang and X. Wang. Deep learning assisted jet tomography for the study of Mach cones in QGP. Unpublished report. (LA-UR-22-29796)

Lee, C., E. Mereghetti, I. M. Vitev, R. Gupta, J. D. Terry, O. S. Tomalak, P. Petreczky, E. T. A. Working Group and W. Ke. The case for an EIC Theory Alliance. Unpublished report. (LA-UR-23-23003)

Xie, M., W. Ke, H. Zhang and X. Wang. Information field based global Bayesian inference of the jet transport coefficient. Unpublished report. (LA-UR-22-25147)

Presentation Slides

Ke, W. Bayesian inference in high-energy nuclear physics. Presented at *The 9th HuaDa QCD School 2021 (Online)*, Wuhan, China, 2021-10-11 - 2021-10-15. (LA-UR-22-29734)

Ke, W. Understanding Nuclear Matter with Jet Physics and Statistics. Presented at *Central China Normal University 2021 International Young Scholars Forum (Online)*, Wuhan, China, 2021-10-23 - 2021-10-26. (LA-UR-22-29737)

Ke, W. eHIJING: the study of in-medium jet fragmentation in e-A. Presented at *The 2rd EicC CDR Workshop (Online)*, Hefei, China, 2022-03-26 - 2022-03-27. (LA-UR-22-29732)

Ke, W. Jet tomography of hot and cold nuclear matter. . (LA-UR-22-29736)

Ke, W. TRENTo initial condition model and the isobar collisions. Presented at *RBRC virtual Workshop, Physics Opportunities from the RHIC Isobar Run (online)*, New York, New York, United States, 2022-01-25 - 2022-01-28. (LA-UR-22-29740)

Ke, W. Heavy-flavor jet modifications in dense QCD medium. Presented at *The 8th International Workshop on Heavy Flavour Production in Nuclear Collisions*, Torino, Italy, 2022-07-14 - 2022-07-16. (LA-UR-22-29741)

Ke, W. Heavy flavor probes of initial & final-state nuclear effects (with emphasis in small systems). Presented at *The 9th Workshop for Early Career Heavy-Ion Physicists*, Estes Park, Colorado, United States, 2022-10-11 - 2022-10-17. (LA-UR-22-30576)

Ke, W. Dynamics of QCD hard probes in eA and pA collisions. Presented at *Triangle Nuclear Theory Colloquium (TNT)*, Durham, North Carolina, United States, 2023-02-14 - 2023-02-14. (LA-UR-23-21844)

Ke, W. Hard probes in isobar collisions & nuclear structures. Presented at *Intersection of nuclear structure and high-energy nuclear collisions, INT 23-1a program (week 2)*, Seattle, Washington, United States, 2023-01-30 - 2023-01-30. (LA-UR-23-21843)

Ke, W. Constraining nuclear structures with hard probes in nuclear collisions. Presented at *Physics Colloquium at East Carolina University*, Greenville, North Carolina, United States, 2023-02-17 - 2023-02-17. (LA-UR-23-21845)

Ke, W., M. Xie, H. Zhang and X. Wang. Functional inference with information field method and application to jet quenching. Presented at *LANL T-2 seminar*, Los Alamos, New Mexico, United States, 2022-11-15 - 2022-11-15. (LA-UR-22-32015)

Ke, W., M. Xie, X. Wang and H. Zhang. Uncovering the temperature dependence of the QGP jet transport parameter using the information field. Presented at *The Berkeley Symposium on Hard Probes and Beyond*, Berkeley, California, United States, 2022-08-18 - 2022-08-19. (LA-UR-22-29738)

Ke, W., M. Xie, X. Wang and H. Zhang. Bayesian analysis with information field approach & application to T -dependent jet transport parameter. Presented at *The 2022 Fall Meeting of the Division of Nuclear Physics of the American Physical Society*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-30. (LA-UR-22-31535)

Ke, W., Y. He, H. Xing, X. Wang and Y. Zhang. Jet tomography in electron-ion collisions. Presented at *Online Seminar at Shandong University & Key Laboratory of Particle Physics and Irradiation*, Qingdao, China, 2022-01-07 - 2022-01-07. (LA-UR-22-29797)

Ke, W. and I. M. Vitev. Heavy-flavor production in dense QCD matter. Presented at *The 29th International Workshop on Deep-Inelastic Scattering & Related Subjects*, Santiago de Compostela, Spain, 2022-05-02 - 2022-05-06. (LA-UR-22-29735)

Ke, W. and I. M. Vitev. A renormalization group analysis of medium-modified fragmentation in SIDIS. Presented at *The 30th International Workshops on Deep-Inelastic Scattering (DIS) and Related Subjects.*, East Lansing, Michigan, United States, 2023-03-27 - 2023-03-31. (LA-UR-23-23117)

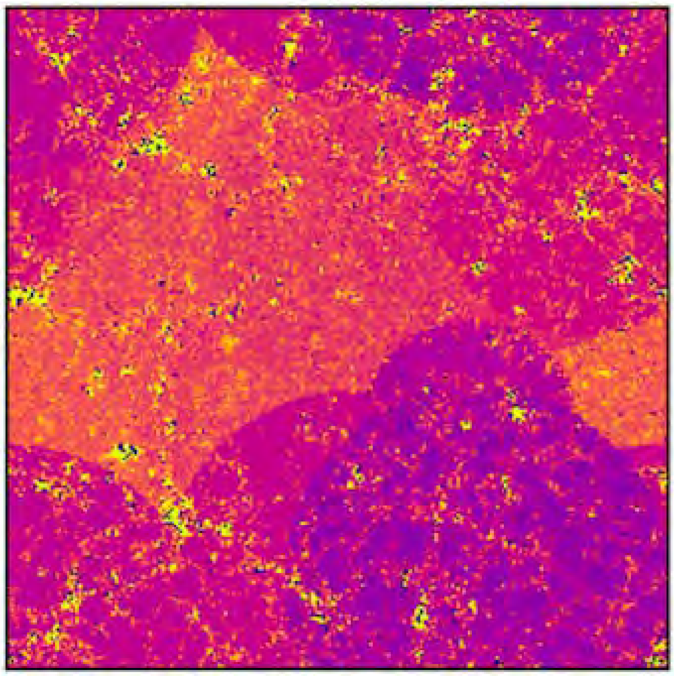
Ke, W. and X. Wang. Combined constraints from jet and hadron quenching to "qhat". Presented at *the XXIXth International Conference on Ultra-relativistic Nucleus-Nucleus Collisions*, Krakow, Poland, 2022-04-04 - 2022-04-10. (LA-UR-22-29784)

Ke, W. and Y. Yin. Extending Hydrodynamic Description of Quark-Gluon Plasm. Presented at *Seminar Series: "Vanderbilt Initiative for Gravity, Waves and Fluids"*, Nashville, Tennessee, United States, 2022-09-15 - 2022-09-15. (LA-UR-22-29733)

**Peer-reviewed*

Supermassive Black Holes and Their Environment

Jarrett Johnson
20210942PRD2



The high energy radiation from the first stars and galaxies heats the universe in an inhomogeneous manner, with some regions experiencing dramatic heating and others remain relatively cold. In this project, the team is modeling the impact this has on the formation and growth of supermassive black holes.

Project Description

The Universe shows us a history that begins with a nearly uniform landscape of gas and dark matter that evolves into a field of non-linear and complex galaxies. A key component of galaxy formation is the seeding and growth of supermassive black holes, now confirmed to exist at the center of nearly all large galaxies. Understanding how these objects form would answer one of most pressing astrophysical questions of the last several decades: Must we invoke new physics to explain the existence of supermassive black holes at early times? This research will provide a theoretical understanding of black hole growth via the interaction between supermassive black holes (SMBHs) and their gaseous environments. It will (1) show that there are observational signatures of primordial black holes as SMBH seeds and (2) determine the impact of radiation from the first galaxies on SMBH assembly. Multiscale modeling of challenging astrophysical problems, like this one, builds capabilty for modeling of the high-energy density environment of nuclear explosions.

Publications

Journal Articles

*Fryer, C. L., A. Y. Lien, A. Fruchter, G. Ghirlanda, D. Hartmann, R. Salvaterra, P. R. U. Sanderbeck and J. L. Johnson. Properties of High-redshift Gamma-Ray Bursts. 2022. *The Astrophysical Journal*. **929** (2): 111. (LA-UR-22-31690 DOI: 10.3847/1538-4357/ac5d5c)

*Johnson, J. L. and P. R. U. Sanderbeck. A Simple Condition for Sustained Super-Eddington Black Hole Growth. 2022. *The Astrophysical Journal*. **934** (1): 58. (LA-UR-22-20494 DOI: 10.3847/1538-4357/ac7b81)

*Sanderbeck, P. U., S. Bird and Z. Haiman. Nucleosynthetic signatures of primordial origin around supermassive black holes. 2021. *Physical Review D*. **104** (10): 103022. (LA-UR-21-30107 DOI: 10.1103/PhysRevD.104.103022)

Presentation Slides

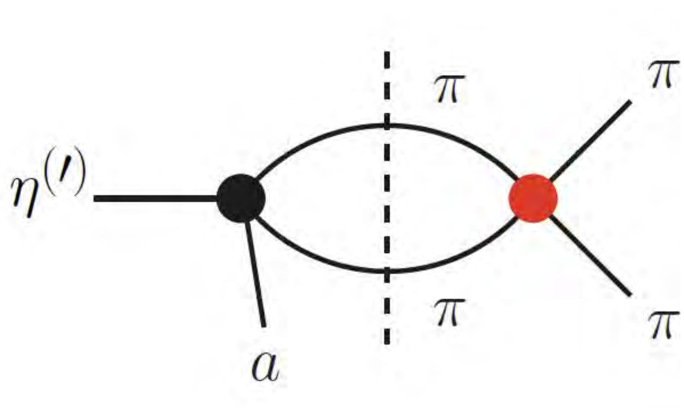
Upton Sanderbeck, P. R. Signatures of primordial origins around supermassive black holes. . (LA-UR-22-20491)

Upton Sanderbeck, P. R. HeII reionization in simulations + (SMBH growth and reionization). Presented at *Reionization and Cosmic Dawn: Looking Forward to the Past*, Berkeley, California, United States, 2022-03-21 - 2022-03-23. (LA-UR-22-22457)

**Peer-reviewed*

Hadronic Physics for Fundamental Discoveries

Daniele Spier Moreira Alves
20210944PRD2



Feynman diagram representing the two-pion intermediate state contribution to the discontinuity of the eta/eta-prime decay into an axion and two pions. Inserting the discontinuity into a dispersion relation one obtains a representation of the amplitude containing the universal, strong pion-pion rescattering effects. Controlling such hadronic effects in this and other similar processes is one of the main goals of this project in order to obtain robust theoretical predictions and interpret experimental data searching for physics beyond the Standard Model in low energy hadronic processes.

Project Description

This project addresses challenges defined as high priority scientific goals by: - The Department of Energy (DOE) Office of Science Particle Physics Project Prioritization Panel (a subpanel of the High Energy Physics Advisory Panel); - The DOE Office of Science Nuclear Physics Long-Range Plan; - The Laboratory's Strategic Investment Priorities under the Nuclear and Particle Futures' Science pillar. These scientific goals refer to the exploration of new particles, interactions, and physical principles. The new particles to be investigated in this project are ""axion-like"" particles and ""hidden photons,"" which are hypothesized new elementary particles predicted by several theories explaining the dark matter in the Universe. This project will calculate the interactions and signals of these new particles in experimental phenomena called ""low energy hadronic processes''. The reason to look into this type of phenomena is the current and near future accumulation of high volume and high quality data. This project will provide robust theoretical foundations to analyze these new experimental data, and shed light on fundamental principles governing elementary particles.

Publications

Journal Articles

Gonzalez-Solis de la Fuente, S. Novel approaches in hadron spectroscopy. 2022. *Progress in Particle and Nuclear Physics*. 103981. (LA-UR-21-31664 DOI: 10.1016/j.ppnp.2022.103981)

Gonzalez-Solis de la Fuente, S. Triangle rescattering in a Feynman integral approach. Submitted to *Physical Review D*. (LA-UR-21-32356)

Gonzalez-Solis de la Fuente, S. Analysis of the doubly radiative decays $\\eta^{(\\prime)}\\to\\pi^0\\gamma\\gamma $ and $\\eta^\\prime\\to\\eta\\gamma\\gamma $. Submitted to *PoS - Proceedings of Science*. (LA-UR-22-22732)

Gonzalez-Solis de la Fuente, S. Exclusive |Vub| determinations using Pad\xc3\xa9 Approximants. Submitted to *PoS - Proceedings of Science*. (LA-UR-22-22737 DOI: 10.22323/1.411.0064)

Gonzalez-Solis de la Fuente, S., R. Escribano and E. Royo. Sensitivity of the and decays to a sub-GeV leptophobic boson. 2022. *Physical Review D*. **106** (11): 114007. (LA-UR-22-26889 DOI: 10.1103/PhysRevD.106.114007)

Reports

Gonzalez-Solis de la Fuente, S., C. Gatto, D. Spier Moreira Alves and S. Pastore. The REDTOP experiment: Rare eta/eta' Decays To Probe New Physics. Unpublished report. (LA-UR-22-22208)

Presentation Slides

Gonzalez-Solis de la Fuente, S. Eta and eta' decays: theory perspective. Presented at *Sergi Gonzalez-Solis*, Cincinnati, Ohio, United States, 2022-05-16 - 2022-05-19. (LA-UR-22-24633)

Gonzalez-Solis de la Fuente, S. Phenomenological applications of Khuri-Treiman equations. Presented at *Invited seminar at Cinvestav*, Mexico city, Mexico, 2022-08-29 - 2022-08-31. (LA-UR-22-29051)

Gonzalez-Solis de la Fuente, S. Phenomenological applications of Khuri-Treiman equations. Presented at *4th Workshop on Future Directions in Spectroscopy Analysis (FDSA2022)*, Newport news, Virginia, United States, 2022-11-14 - 2022-11-16. (LA-UR-22-31975)

Gonzalez-Solis de la Fuente, S. Sensitivity of the $\\eta^{(\\prime)}\\to\\pi^{0}\\gamma\\gamma$ and $\\eta^{\\prime}\\to\\eta\\gamma\\gamma$ decays to a sub-GeV leptophobic $U(1)_{B}$ boson. . (LA-UR-22-32244)

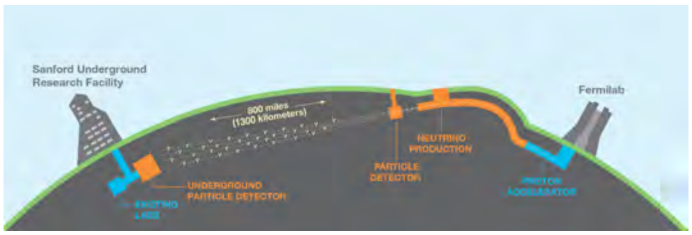
Gonzalez-Solis de la Fuente, S. Exclusive $|V_{ub}|$ determinations\\\\ using Pad\\'{e} Approximants. Presented at *Seminar at the University of Arizona*, Tucson, Arizona, United States, 2023-02-08 - 2023-02-08. (LA-UR-23-21297)

**Peer-reviewed*

Radiative Corrections for the Discovery of Charge-Parity Violation in the Lepton Sector

Ivan Vitev

20210968PRD4



In the Deep Underground Neutrino Experiment, beams of neutrinos and antineutrinos will travel 800 miles from Fermilab to Sanford Underground Research Facility, South Dakota. This project will provide the theoretical input to determine the fluxes of outgoing neutrinos and to reconstruct the energy of the neutrinos when they hit the far detector in South Dakota.

Project Description

Understanding whether the laws of nature are symmetric under the interchange of particles and antiparticles is a key open question in science and is a key driver in the Department of Energy Office of Science mission in both High Energy Physics and Nuclear Physics. This project will address theoretical challenges related to the interpretation of the next-generation flagship project called Deep Underground Neutrino Experiment, aimed to uncover whether neutrinos and antineutrinos obey exactly the same physical laws. This project will provide high-precision calculation of neutrino-initiated reactions needed to assess the behavior of neutrinos and antineutrinos.

Publications

Journal Articles

Alioli, S. and O. S. Tomalak. Event Generators for High-Energy Physics Experiments. Submitted to *Snowmass White Paper*. (LA-UR-22-22126)

Mereghetti, E., K. Quirion, E. Passemar and O. S. Tomalak. Notes on pion electron- and neutrino-production amplitudes. Submitted to *most likely PRD after a lot of work*. (LA-UR-22-22740)

*Tomalak, O. Radiative (anti)neutrino energy spectra from muon, pion, and kaon decays. 2002. *Physics Letters B*. **829**: 137108. (LA-UR-21-30638 DOI: 10.1016/j.physletb.2022.137108)

Tomalak, O. S. Coulomb corrections for lepton-nucleus scattering with soft collinear effective theory. Submitted to *PRD or JHEP*. (LA-UR-21-30633)

Tomalak, O. S. Radiative corrections to inverse muon decay for accelerator neutrinos. Submitted to *PRD*. (LA-UR-22-29964)

Tomalak, O. S., A. Afanasev, A. Schmidt , J. Bernauer , E. Cline, F. Hagelstein, V. Sharkovska, E. Tomasi-Gustafsson, F. Myhrer and P. Blunden. Two-photon exchange in lepton-proton scattering. Submitted to *European Physical Journal A. Hadrons and Nuclei*. (LA-UR-22-32680)

Tomalak, O. S., E. Mereghetti and V. Cirigliano. Notes on two-step matching from the Standard Model high-energy to the four-Fermi theory and to the ChPT at low energy. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics; after the work is done*. (LA-UR-22-21034)

Tomalak, O. S., P. B. Denton, A. Aurisano, M. Bishai, A. De Gouvea, I. Mocioiu, J. Gehrlein, S. Wissel, A. De Roeck and G. Working. Tau Neutrinos in the Next Decade: from GeV to EeV. Submitted to *J.Phys.G*. (LA-UR-21-32255)

Tomalak, O. S., Q. Chen, R. J. Hill, K. S. McFarland and C. Wret. Theory of QED radiative corrections to neutrino scattering at accelerator energies. Submitted to *Phys.Rev.D 106, 9, 093006 (2022)*. (LA-UR-21-30632)

Tomalak, O. S., R. Petti and R. J. Hill. Nucleon axial radius and form factor with future neutrino experiments. Submitted to *discussed upon completion, PRD or PRC are among the options*. (LA-UR-22-32611)

Tomalak, O. S. and I. M. Vitev. Coulomb corrections and exchange of Glauber photons in neutrino-nucleus scattering. Submitted to *Depends what comes out*. (LA-UR-21-30814)

Tomalak, O. S. and I. M. Vitev. QED medium effects in (anti)neutrino-nucleus and electron-nucleus scattering: Elastic scattering on nucleons. Submitted to *Phys.Lett.B 835 (2022) 137492*. (LA-UR-22-22739)

*Tomalak, O., Q. Chen, R. J. Hill and K. S. McFarland. QED radiative corrections for accelerator neutrinos. 2022. *Nature Communications*. **13** (1): 5286. (LA-UR-21-27844 DOI: 10.1038/s41467-022-32974-x)

Reports

Lee, C., E. Mereghetti, I. M. Vitev, R. Gupta, J. D. Terry, O. S. Tomalak, P. Petreczky, E. T. A. Working Group and W. Ke. The case for an EIC Theory Alliance. Unpublished report. (LA-UR-23-23003)

Alvarez Ruso, L., T. Bhattacharya, J. A. Carlson, O. S. Tomalak and R. Gupta. Theoretical tools for neutrino scattering: interplay between lattice QCD, EFTs, nuclear physics, phenomenology, and neutrino event generators. Unpublished report. (LA-UR-22-22647)

Tomalak, O. S. Neutrino Scattering Measurements on Hydrogen and Deuterium: A Snowmass White Paper. Unpublished report. (LA-UR-21-31459)

Presentation Slides

Tomalak, O. S. Radiative corrections in electron and neutrino scattering. Presented at *Neutrinos as a Portal to New Physics and Astrophysics*, Santa Barbara, California, United States, 2022-02-14 - 2022-03-31. (LA-UR-22-21241)

Tomalak, O. S. Radiative corrections. Presented at *NuSTEC Workshop on Electron Scattering*, Tel Aviv, Israel, 2022-03-28 - 2022-04-01. (LA-UR-22-22434)

Tomalak, O. S. Radiative corrections to charged-current neutrino scattering at GeV energies. Presented at *The XIXth annual workshop on Soft-Collinear Effective Theory 2022*, Bern, Switzerland, 2022-04-19 - 2022-04-22. (LA-UR-22-23396)

Tomalak, O. S. QED nuclear medium effects in lepton-nucleus scattering. Presented at *International Conference on High Energy Physics*, Bolgna, Italy, 2022-07-06 - 2022-06-13. (LA-UR-22-25980)

Tomalak, O. S. QED nuclear medium effects in neutrino-nucleus and electron-nucleus scattering. Presented at *PASCOS 2022, the 27th International Symposium on Particles, Strings and Cosmology*, Heidelberg, Germany, 2022-07-25 - 2022-07-29. (LA-UR-22-25998)

Tomalak, O. S. Radiative corrections to charged-current neutrino scattering at GeV energies. Presented at *Radiative Corrections from medium to high energy experiments*, Trento, Italy, 2022-07-18 - 2022-07-22. (LA-UR-22-25962)

Tomalak, O. S. An Overview of Cross Sections in Neutrino Physics. Presented at *14th Conference on the Intersections of Particle and Nuclear Physics (CIPANP 2022)*, Orlando, Florida, United States, 2022-08-29 - 2022-09-04. (LA-UR-22-28913)

Tomalak, O. S. QED radiative corrections and nuclear medium effects at GeV energies. Presented at *NuINT 2022*, Seoul, Korea, South, 2022-10-24 - 2022-10-29. (LA-UR-22-29360)

Tomalak, O. S. Axial and pseudoscalar form factors from charged-current neutrino-nucleon elastic scattering. Presented at *2021 Fall Meeting of the APS DNP, virtual*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-29985)

Tomalak, O. S. QED radiative corrections to charged-current neutrino-nucleon elastic scattering for accelerator neutrino experiment. Presented at *NuFact 2021: The 22nd International Workshop on Neutrinos from Accelerators*, Cagliari, Italy, 2021-09-05 - 2021-09-11. (LA-UR-21-28076)

Tomalak, O. S. QED radiative corrections to charged-current neutrino-nucleon elastic scattering for accelerator neutrino experiments. Presented at *FNAL Neutrino Joint Theory-Experiment Working Group Meeting*, Batavia, Illinois, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-29212)

Tomalak, O. S. Radiative corrections to neutron beta decay from low-energy effective field theory. Presented at *The 2022 International Conference on the Structure of Baryons, Baryons-2022*, Sevilla, Spain, 2022-11-07 - 2022-11-11. (LA-UR-22-31609)

Tomalak, O. S. Radiative corrections to neutron beta decay from low-energy effective field theory. Presented at *The 2022 International Conference on the Structure of Baryons, Baryons-2022*, Sevilla, Spain, 2022-11-07 - 2022-11-11. (LA-UR-23-20003)

Tomalak, O. S. Radiative corrections in neutrino physics. Presented at *S@INT Seminar Series*, Seattle, Washington, United States, 2023-01-19 - 2023-01-19. (LA-UR-23-20009)

Tomalak, O. S. Radiative corrections for precise low- and high-energy (anti)neutrino flux constraints. Presented at *DIS 2023*, East Lansing, Michigan, United States, 2023-03-29 - 2023-03-31. (LA-UR-23-22298)

Tomalak, O. S. Status of proton radius puzzle and QED radiative corrections for accelerator neutrinos. Presented at *Seminar at KIAS*, Seoul, Korea, South, 2023-04-05 - 2023-04-14. (LA-UR-23-22299)

Tomalak, O. S. QED radiative corrections for accelerator neutrinos. Presented at *Seminar at Institute for Nuclear Physics, Mainz, Germany*, Mainz, Germany, 2023-03-20 - 2023-03-21. (LA-UR-23-22296)

Tomalak, O. S. Radiative corrections to low-energy neutral-current neutrino scattering and DAR sources. Presented at *The Magnificent CEvNS 2023 Workshop*, Munich, Germany, 2023-03-22 - 2023-03-23. (LA-UR-23-22297)

Tomalak, O. S. QED radiative corrections for accelerator neutrinos.. Presented at *XXth Workshop of Soft Collinear Effective Theory*, Berkeley, California, United States, 2023-03-27 - 2023-03-31. (LA-UR-23-23037)

Tomalak, O. S. Radiative corrections in electron and neutrino physics. Presented at *Seminar at JLab Theory Center*, Newport News, Virginia, United States, 2023-04-05 - 2023-04-05. (LA-UR-23-23044)

Tomalak, O. S. Theory and experiment for precision neutrino physics. Presented at *Physics Colloquium at Old Dominion University*, Norfolk, Virginia, United States, 2023-04-06 - 2023-04-06. (LA-UR-23-23048)

Tomalak, O. S. Radiative corrections to low-energy neutral-current neutrino scattering and DAR sources. Presented at *Interplay of Nuclear, Neutrino and BSM Physics at Low-Energies"*, Seattle, Washington, United States, 2023-04-17 - 2023-04-21. (LA-UR-23-23047)

Tomalak, O. S. and A. Afanasev. Radiative Corrections for Proton Radius Measurements: Scattering Experiments. Presented at *PREN 2022 Convention International STRONG-2020 Workshop on the Proton Charge Radius and related topics*, Paris, France, 2022-06-20 - 2022-06-23. (LA-UR-22-25710)

Posters

Tomalak, O. S. QED corrections to charged-current neutrino-nucleon elastic scattering. Presented at *The XXX International Conference on Neutrino Physics and Astrophysics*, Seoul, Korea, South, 2022-05-30 - 2022-06-04. (LA-UR-22-23397)

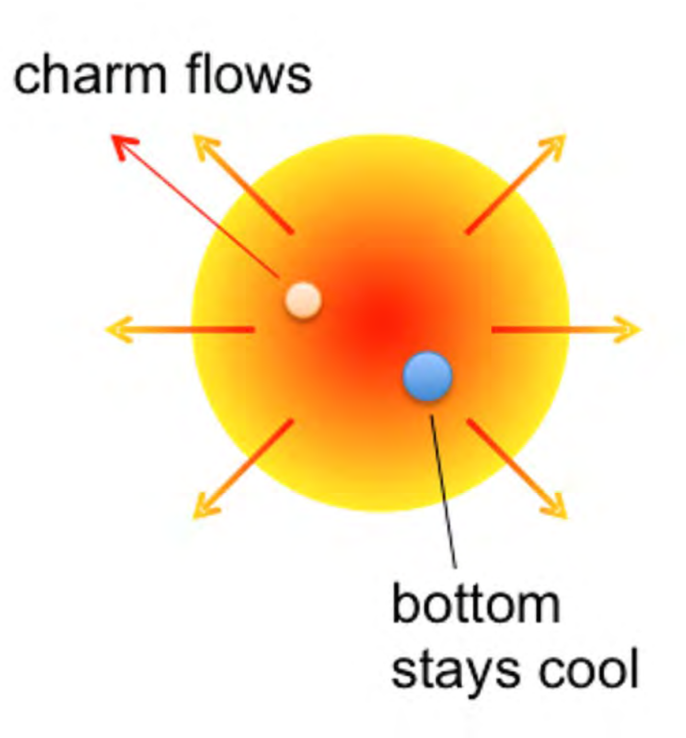
Tomalak, O. S. QED corrections to charged-current neutrino-nucleon elastic scattering. Presented at *PANIC 2021: Particles and Nuclei International Conference*, Lisbon, Portugal, 2021-08-05 - 2021-08-10. (LA-UR-21-28153)

Tomalak, O. S. and I. M. Vitev. QED nuclear medium effects in neutrino-nucleus and electron-nucleus scattering. Presented at *Quark Matter 2022*, Krakow, Poland, 2022-04-04 - 2022-04-10. (LA-UR-22-22741)

**Peer-reviewed*

Probing the Fundamental Properties of Quark-Gluon Plasma with Heavy Quarks

Ming Liu
20220698PRD1



The interactions of the charm and bottom quarks inside the QGP created in heavy ion collisions. The less-heavy charm quark flows with the hot and dense QGP medium while the motion of the much heavier bottom quark will be less affected the the QGP. We will construct state-of-the-art AI-ML based tools to detect one of the heaviest subatomic particles (b-hadrons) produced in heavy ion collisions to study Quark-gluon plasma (QGP) created in high energy heavy ion collisions at physics detector experiments sPHENIX and Large Hadron Collider beauty (LHCb).

Project Description

The goal of this project is to address important physics questions in Quark-Gluon-Plasma (QGP) physics using a new artificial intelligence-machine learning based algorithm to identify rare events in the sPHENIX experiment (strongly interacting particles and use of the Pioneering High Energy Nulcear Interaction eXperiment) at the Relativistic Heavy Ion Collider (RHIC) at the Brookhaven National Lab. Measurements of modification of heavy quark production in high energy heavy ion collisions at RHIC and large hadron collider (LHC) will help us to understand various quark energy loss mechanisms, including radiative and collisional energy loss inside the QGP. This project will make it possible to address key aspects of heavy quark physics at the next generation heavy ion experiment in the United States, the sPHENIX experiment.

Publications

Presentation Slides

Shi, Z. AI/ML Heavy Flavor trigger at EIC. Presented at *Exotic heavy meson spectroscopy and structure with EIC*, STONY BROOK, New York, United States, 2022-08-15 - 2022-08-18. (LA-UR-22-28826)

Shi, Z. The sPHENIX Open and Close Heavy Flavor Program. Presented at *The 9th International Conference on Quarks and Nuclear Physics*, Tallahassee, Florida, United States, 2022-09-05 - 2022-09-09. (LA-UR-22-29200)

Shi, Z. Investigation of Beauty Hadronization Universality from Vacuum to QGP. Presented at *Advancing the Understanding of Non-Perturbative QCD Using Energy Flows*, STONY BROOK, New York, United States, 2022-09-19 - 2022-09-22. (LA-UR-22-30134)

Shi, Z. sPHENIX Heavy Flavor Physics Simulation Performance. Presented at *2022 Fall Meeting of the APS Division of Nuclear Physics*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-30. (LA-UR-22-31007)

Shi, Z. Measurements of J/\xcf\x88 Production vs Event Multiplicity in the Forward Rapidity in p + p Collisions in the PHENIX Experiment. Presented at *22nd Zim\xc3\xa1nyi School Winter Workshop on Heavy Ion Physics*, Budapest, Hungary, 2022-12-05 - 2022-12-09. (LA-UR-23-20973)

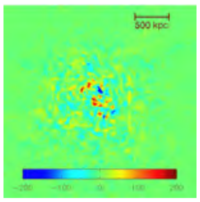
Shi, Z., C. Woody, J. Lajoie and I. Delk. Development of Future Electromagnetic Calorimeter Technologies and Applications for the Electron-Ion Collider with GEANT 4 Simulations. Presented at *The 20th International Conference on Strangeness in Quark Matter*, Busan, Korea, South, 2022-06-13 - 2022-06-17. (LA-UR-22-26601)

Shi, Z. and M. X. Liu. Measurements of J/\xcf\x88 production vs event multiplicity in the forward rapidity in p + p and p + Au collisions in the PHENIX experiment. Presented at *2022 Fall Meeting of the APS Division of Nuclear Physics*, New Orleans, Louisiana, United States, 2022-10-27 - 2022-10-30. (LA-UR-23-20996)

**Peer-reviewed*

New Methods to Determine Magnetic Field Conditions in Galaxy Clusters and Cosmology

Hui Li
20220700PRD1



Understanding magnetic fields in galaxy clusters is challenging because it is difficult to measure the magnetic field through observations. New techniques are being developed to infer the magnetic field strength and configuration using the variations and gradients in intensity and polarization. Such new techniques will be tested and validated using extensive magnetohydrodynamics simulations of galaxy clusters. One such simulation is shown in this figure depicting the integrated Faraday Rotation Measurement with patches indicating spatial variations and turbulence. Once confirmed, these new techniques will enable advanced understanding and evaluation of magnetic fields in cosmology. [Image credit: Los Alamos National Laboratory]

Project Description

Such a systematic and accurate study of magnetic field morphology and strength in the Intra-Cluster Medium will be the first of its kind and its outcome will provide the much-needed information for cosmological structure formation studies. This proposal places Los Alamos National Laboratory in a strong position preparing for the emerging science enabled by the next-generation telescopes such as Square Kilometer Array.

Publications

Journal Articles

Ho, K. W., K. H. Yuen and A. Lazarian. How the existence of unstable neutral media restricts the aspect ratio of cold neutral media?. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-22-28584)

Malik, S., K. H. Yuen and H. Yan. Diagnosis of 3D magnetic field and modes composition in MHD turbulence with Y-parameter. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-23-23203)

Yuen, K. H., H. Yan and A. Lazarian. Anomalous compressible mode generation by global frame projections of pure Alfven mode. 2023. *Monthly Notices of the Royal Astronomical Society*. (LA-UR-22-28314 DOI: 10.1093/mnras/stad287)

Yuen, K. H., K. W. Ho, C. Y. Law, A. Chen and A. Lazarian. Turbulent universal galactic Kolmogorov velocity cascade over 6 decades. Submitted to *Nature Communications*. (LA-UR-22-28682)

Zhao, S., H. Yan, T. Z. Liu, K. H. Yuen and H. Wang. Satellite observations of the Alfv\xc3\xa9nic 1 Transition from Weak to Strong Magnetohydrodynamic Turbulence. Submitted to *Nature Physics*. (LA-UR-22-32817)

Reports

Malik, S., K. H. Yuen, P. Pavaskar and H. Yan. Study of turbulent universe: anisotropy analysis. Unpublished report. (LA-UR-23-20568)

Yan, H., K. H. Yuen, S. Malik and P. Pavaskar. Mode classification in magnetized ISM turbulence. Unpublished report. (LA-UR-23-20569)

Presentation Slides

Yuen, K. H. New Method in Tracing Magnetic Fields in Interstellar Media. Presented at *T-2 seminar*, Los Alamos, New Mexico, United States, 2022-09-22 - 2022-09-22. (LA-UR-22-29571)

Yuen, K. H. Accurate Magnetic Field Strength Estimation via Differential Measure Analysis (DMA). Presented at *Online Seminar by Alex Lazarian.*, Madison, Wisconsin, United States, 2022-09-20 - 2022-09-20. (LA-UR-22-29686)

Yuen, K. H. Origin of magnetically elongated cold neutral media in multiphase interstellar media. Presented at *AAPPS-DPP2022*, Remote, Japan, 2022-10-10 - 2022-10-14. (LA-UR-22-30574)

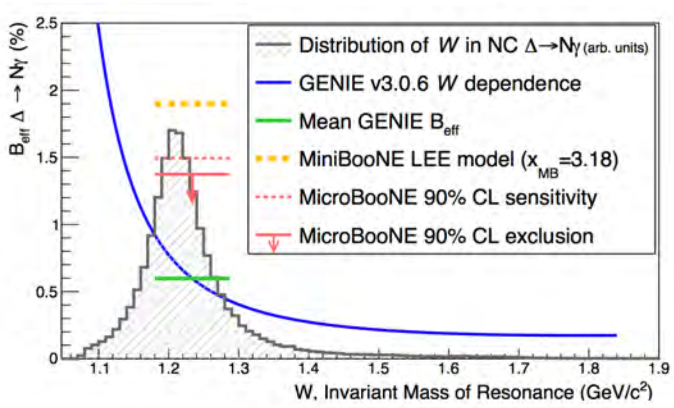
Yuen, K. H. Origin of magnetically elongated cold neutral media in multiphase interstellar media: A simulation perspective. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30822)

Yuen, K. H. Origin of magnetically elongated cold neutral media in multiphase interstellar media. Presented at *20th Annual International Astrophysical Conference*, Santa Fe, New Mexico, United States, 2022-10-31 - 2022-11-04. (LA-UR-22-31461)

**Peer-reviewed*

Unraveling the Mysteries of the Ghostly Neutrino

Mark Ross-Lonergan
20220714PRD1



This figure shows the extracted 90% Confidence Level (CL) on the effective branching fraction for a particular neutrino-induced single gamma production process, neutral current (NC) resonant Delta (1232) baryon production followed by Delta radiative decay. The gray shaded histogram shows the distribution of W, the resonance invariant mass, for all simulated NC Delta to Gamma processes. This result represents the world's most sensitive search to date for the NC Delta process, below 1 giga-electron volt, and a first test of the MiniBooNE (the Cherenkov detector experiment) low-energy excess under a single photon hypothesis. The data rules out the interpretation of the MiniBooNE anomalous excess for this particular enhanced single photon process and opens the door to further searches that focus on a broader range of models such as coherent single-photon production and more exotic beyond-Standard Model processes that manifest as single-photon events, such as co-linear electron-positron pairs from Z' or scalar decays, among others. The discovery of new Beyond the Standard Model particles and interactions would be transformative for high-energy physics, nuclear physics, and astrophysics which is a key mission area for LANL. Reference: arXiv: 2110.00409, Phys. Rev. Lett. 128, 111801 (2022). Credit: MicroBoNE Collaboration

Project Description

This project will address the evidence for physics beyond the Standard Model (BSM) from the short-baseline neutrino anomalies, which may be explained by new fundamental particles and interactions that are part of the dark sector, which comprises 95% of the mass-energy of the universe. By analyzing new data and developing new phenomenological models, the goal of the project is to explain the neutrino anomalies with new BSM physics models, which would have a major impact on high-energy physics, nuclear physics, and astrophysics. This work will also provide important future directions for the upcoming United States-led flagship neutrino experiment, the Deep Underground Neutrino Experiment (DUNE).

Publications

Journal Articles

*Abratenko, P., R. An, J. Anthony, L. Arellano, J. Asaadi, A. Ashkenazi, S. Balasubramanian, B. Baller, C. Barnes, G. Barr, V. Basque, L. Bathe-Peters, O. Benevides Rodrigues, S. Berkman, A. Bhanderi, A. Bhat, M. Bishai, A. Blake, T. Bolton, J. Y. Book, L. Camilleri, D. Caratelli, I. Caro Terrazas, R. Castillo Fernandez, F. Cavanna, G. Cerati, Y. Chen, D. Cianci, J. M. Conrad, M. Convery, L. Cooper-Troendle, J. I. Crespo-Anad\xc3\xb3n, M. Del Tutto, S. R. Dennis, P. Detje, A. Devitt, R. Diurba, R. Dorrill, K. Duffy, S. Dytman, B. Eberly, A. Ereditato, J. J. Evans, R. Fine, G. A. Fiorentini Aguirre, R. S. Fitzpatrick, B. T. Fleming, N. Foppiani, D. Franco, A. P. Furmanski, D. Garcia-Gamez, S. Gardiner, G. Ge, S. Gollapinni, O. Goodwin, E. Gramellini, P. Green, H. Greenlee, W. Gu, R. Guenette, P. Guzowski, L. Hagaman, O. Hen, C. Hilgenberg, G. A. Horton-Smith, A. Hourlier, R. Itay, C. James, X. Ji, L. Jiang, J. H. Jo, R. A. Johnson, Y. -. J. Jwa, D. Kalra, N. Kamp, N. Kaneshige, G. Karagiorgi, W. Ketchum, M. Kirby, T. Kobilarcik, I. Kreslo, R. LaZur, I. Lepetic, K. Li, Y. Li, K. Lin, B. R. Littlejohn, W. C. Louis, X. Luo, K. Manivannan, C. Mariani, D. Marsden, J. Marshall, D. A. Martinez Caicedo, K. Mason, A. Mastbaum, N. McConkey, V. Meddage, T. Mettler, K. Miller, J. Mills, K. Mistry, A. Mogan, T. Mohayai, J. Moon, M. Mooney, A. F. Moor, C. D. Moore, L. Mora Lepin, J. Mousseau, M. Murphy, R. Murrells, D. Naples, A. Navrer-Agasson, M. Nebot-Guinot, R. K. Neely, D. A. Newmark, J. Nowak, M. Nunes, O. Palamara, V. Paolone, A. Papadopoulou, V. Papavassiliou, S. F. Pate, N. Patel, A. Paudel, Z. Pavlovic, E. Piasetzky, I. D. Ponce-Pinto, S. Prince, X. Qian, J. L. Raaf, V. Radeka, A. Rafique, M. Reggiani-Guzzo, L. Ren, L. C. J. Rice, L. Rochester, J. Rodriguez Rondon, M. Rosenberg, M. Ross-Lonergan, G. Scanavini, D. W. Schmitz, A. Schukraft, W. Seligman, M. H. Shaevitz, R. Sharankova, J. Shi, J. Sinclair, A. Smith, E. L. Snider, M. Soderberg, S. S \xc3\xb6ldner-Rembold, P. Spentzouris, J. Spitz, M. Stancari, J. S. John, T. Strauss, K. Sutton, S. Sword-Fehlberg, A. M. Szelc, W. Tang, K. Terao, C. Thorpe, D. Totani, M. Toups, Y. -. T. Tsai, M. A. Uchida, T. Usher, W. Van De Pontseele, B. Viren, M. Weber, H. Wei, Z. Williams, S. Wolbers, T. Wongjirad, M. Wospakrik, K. Wresilo, N. Wright, W. Wu, E. Yandel, T. Yang, G. Yarbrough, L. E. Yates, H. W. Yu, G. P. Zeller, J. Zennamo and C. Zhang. Search for Neutrino-Induced Neutral-Current \xce\x94 Radiative Decay in MicroBooNE and a First Test of the MiniBooNE Low Energy Excess under a Single-Photon Hypothesis. 2022. *Physical Review Letters*. **128** (11): 111801. (LA-UR-22-31532 DOI: 10.1103/PhysRevLett.128.111801)

Presentation Slides

Gollapinni, S. and M. P. Ross-Lonergan. Experimental Status: Atmospheric/Accelerator DIF and DAR. Presented at *Snowmass Community Summer Study Workshop*, Seattle, Washington, United States, 2022-07-17 - 2022-07-26. (LA-UR-22-31518)

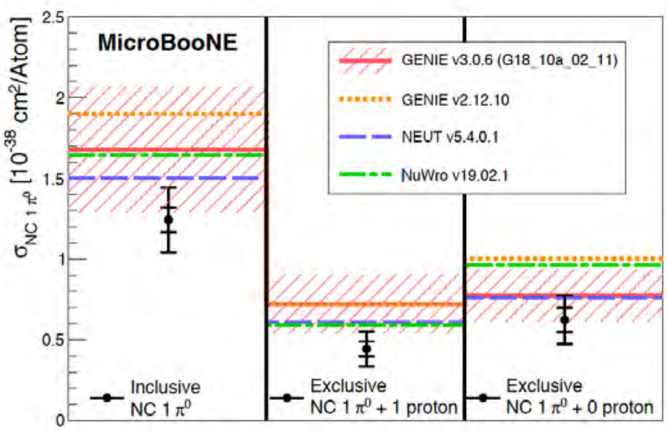
Gollapinni, S. and M. P. Ross-Lonergan. Short Baseline Experiments. Presented at *NuFact 2022: The 23rd International Workshop on Neutrinos from Accelerators*, Snowbird, Utah, United States, 2022-07-31 - 2022-08-06. (LA-UR-22-31520)

Gollapinni, S. and M. P. Ross-Lonergan. Cracking down on neutrino anomalies using liquid argon neutrino detectors. Presented at *LANL Physics Cafe*, Los Alamos, New Mexico, United States, 2022-10-25 - 2022-10-25. (LA-UR-22-31565)

**Peer-reviewed*

Cross Sections on Argon: Enabling the Future of Neutrino Physics

Sowjanya Gollapinni
20220719PRD1



The figure shows the highest statistics measurement to date of neutrino neutral current single pion production on argon, including the first exclusive measurements of this process ever made in argon. Inclusive and exclusive measured cross sections are compared to the simulated cross sections from several neutrino event generators including Generates Events for Neutrino Interaction Experiments (GENIE) along with its uncertainties (shaded red bands), and other contemporary generators such as NuWro (a neutrino event generator developed by the Wrocław Neutrino Group), and NEUT (a neutrino interaction event generator). Reference: https://arxiv.org/pdf/2205.07943.pdf (submitted to Physics Review D). This figure highlights the importance of addressing the critical gap in our current knowledge of how neutrinos interact with argon especially the processes that are key backgrounds in analyses searching for sterile neutrinos and other exotic new physics which is key area of focus under LANL's Nuclear and Particle Futures (NPF) pillar. Credit: MicroBooNE Collaboration

Project Description

Neutrinos are the most elusive fundamental particles that we know of and are at the center of most foundational questions in science today such as "Why do we live in a matter-dominated universe?" and "What is dark matter made of?" Through Micro Booster Neutrino Experiment (MicroBooNE) and the Short-Baseline Neutrino (SBN) program, and the upcoming Deep Underground Neutrino Experiment (DUNE), the particle physics community aims to make most precise measurements ever of neutrino properties and directly test questions surrounding the neutrinos. Success in any of these goals would be a breakthrough result in physics, but each requires that neutrino cross sections on argon be measured to an unprecedented level of precision. This project will address this critical gap in our current knowledge of how neutrinos interact on argon using data from MicroBooNE and SBN. This work will enable a cross section program through the next generation of analyses and to pioneer novel techniques for measuring neutrino-argon interactions especially those that are key background in analyses searching for sterile neutrinos and other exotic new physics. This project will also forge new theory collaborations to deeply probe important neutrino interaction models to improve and constrain nuclear models with state-of-the-art calculations of nuclei.

Publications

Reports

Gollapinni, S., R. D. Fine, N. P. Oza, M. P. Ross-Lonergan and Collaboration MicroBooNE. Measurement of neutral current single \xcf\x800 production on argon with the MicroBooNE detector. Unpublished report. (LA-UR-22-31519)

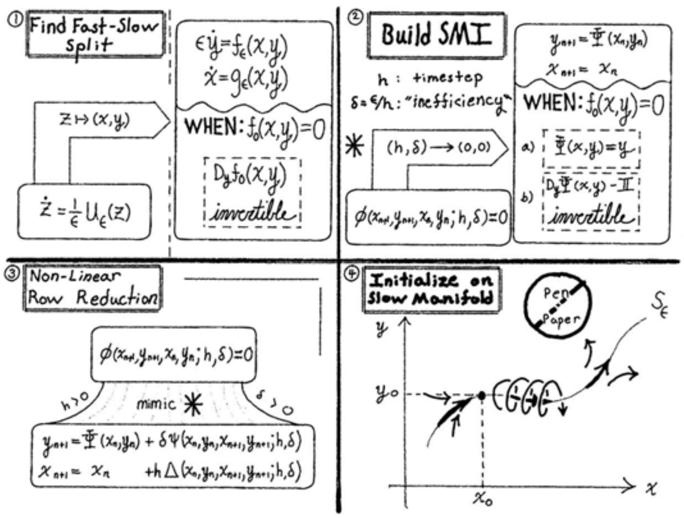
Presentation Slides

Gollapinni, S., R. D. Fine and Collaboration MicroBooNE. Measurements of pion production at MicroBooNE. Presented at *The 13th International Workshop on Neutrino-Nucleus Interactions in the Few GeV Regions*, Seoul, Korea, South, 2022-10-24 - 2022-10-29. (LA-UR-22-31566)

**Peer-reviewed*

Conservative Slow-Manifold Integrators

Joshua Burby
20180756PRD4



Slow manifold integrators comprise a class of implicit time-marching schemes that can accurately step over stiff timescales when applied to solutions that do not sample the fastest dynamics. They function based on the dynamical systems principle of a slow almost-invariant manifold. Knowledge of a continuous-time systems slow manifold structure is exploited in the slow manifold integrator framework to both ensure large-timestep accuracy and resolve the preconditioning issue that commonly plagues implicit schemes.

Project Description

Physical systems and their computational modeling in national security applications often encounter extreme scale separation. The inherent stiffness in the physical models presents a grand challenge in multiscale simulations and predictive science. The current project seeks to develop a new paradigm in multiscale simulations via the so-called conservative slow manifold integrators. The key innovation is based on two fundamental properties of stiff systems that have been largely overlooked by previous investigators: (1) in the presence of irrelevant timescales, dynamics occur on invariant sets known as slow manifolds; (2) systems with conservation laws aways possess multi-linear skew-symmetric brackets that generalize Poisson brackets. Through the identification of slow manifolds, we can systematically identify dependent variables for various systems that nonlinearly separate the relevant and irrelevant timescales. In terms of those variables, we will then discretize the relevant skew-symmetric bracket in order to derive nonlinearly-implicit time integrators that preserve any number of first integrals exactly. This new advance will lead to groundbreaking simulations for topical problems in magnetic and inertial confinement fusion physics where the numerical and physical implications of stiffness are poorly understood.

Technical Outcomes

This project successfully developed conservative slow manifold integration (CSMI). CSMI geometrically interprets numerically "stepping over" short timescales. Project results revealed when large implicit timesteps make or don't make sense; was able to systematize preconditioning nonlinear implicit timesteps and synthesize integration techniques for non-dissipative systems, like symplectic integration, with the implicit timestepping framework. CSMI uncovered a deleterious numerical instability that affects non-dissipative implicit integration schemes. The project resolved the instability problem for many physical systems.

Publications

Journal Articles

*Burby, J. W. Guiding center dynamics as motion on a formal slow manifold in loop space. 2020. *Journal of Mathematical Physics*. **61** (1): 12703. (LA-UR-19-24299 DOI: 10.1063/1.5119801)

*Burby, J. W. Slow manifold reduction as a systematic tool for revealing the geometry of phase space. 2022. *Physics of Plasmas*. **29** (4): 042102. (LA-UR-22-20125 DOI: 10.1063/5.0084543)

Burby, J. W., E. Hirvijoki and M. Leok. Nearly-periodic maps and geometric integration of noncanonical Hamiltonian systems. Submitted to *Journal of Nonlinear Science*. (LA-UR-21-32231)

*Burby, J. W., J. M. Finn and C. L. Ellison. Improved accuracy in degenerate variational integrators for guiding centre and magnetic field line flow. 2022. *Journal of Plasma Physics*. **88** (2): 835880201. (LA-UR-21-22168 DOI: 10.1017/S0022377821001136)

*Burby, J. W., N. Duignan and J. D. Meiss. Integrability, normal forms, and magnetic axis coordinates. 2021. *Journal of Mathematical Physics*. **62** (12): 122901. (LA-UR-21-22030 DOI: 10.1063/5.0049361)

Burby, J. W., N. Duignan and J. Meiss. Minimizing Separatrix Crossings through Isoprominence. Submitted to *Plasma Physics and Controlled Fusion*. (LA-UR-22-30857)

*Burby, J. W., N. Kallinikos and R. MacKay. Generalized Grad–Shafranov equation for non-axisymmetric MHD equilibria. 2020. *Physics of Plasmas*. **27** (10): 102504. (LA-UR-20-24232 DOI: 10.1063/5.0015420)

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*Burby, J. W., Q. Tang and R. Maulik. Fast neural Poincar\xc3\xa9 maps for toroidal magnetic fields. 2021. *Plasma Physics and Controlled Fusion*. **63** (2): 24001. (LA-UR-20-25019 DOI: 10.1088/1361-6587/abcbaa)

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*Burby, J. W. and D. E. Ruiz. Variational nonlinear WKB in the Eulerian frame. 2020. *Journal of Mathematical Physics*. **61** (5): 53101. (LA-UR-19-21078 DOI: 10.1063/1.5099383)

*Burby, J. W. and E. Hirvijoki. Normal stability of slow manifolds in nearly periodic Hamiltonian systems. 2021. *Journal of Mathematical Physics*. **62** (9): 093506. (LA-UR-21-23132 DOI: 10.1063/5.0054323)

Burby, J. W. and J. Squire. General formulas for adiabatic invariants in nearly-periodic Hamiltonian systems. Submitted to *Journal of Plasma Physics*. (LA-UR-20-23640)

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*Hirvijoki, E., J. W. Burby, D. Pfefferle and A. J. Brizard. Energy and momentum conservation in the Euler–Poincar\xc3\xa9 formulation of local Vlasov–Maxwell-type systems. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (23): 235204. (LA-UR-19-32412 DOI: 10.1088/1751-8121/ab8b38)

Hirvijoki, E., J. W. Burby and A. J. Brizard. Metriplectic foundations of gyrokinetic Vlasov-Maxwell-Landau theory. Submitted to *Physical Review Letters*. (LA-UR-22-21790)

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*Miloshevich, G. and J. W. Burby. Hamiltonian reduction of Vlasov-Maxwell to a dark slow manifold. 2021. *Journal of Plasma Physics*. **87** (3): 835870301. (LA-UR-21-20381 DOI: 10.1017/S0022377821000556)

*Parker, J. B., J. W. Burby, J. B. Marston and S. M. Tobias. Nontrivial topology in the continuous spectrum of a magnetized plasma. 2020. *Physical Review Research*. **2** (3): 033425. (LA-UR-20-28556 DOI: 10.1103/PhysRevResearch.2.033425)

Zonta, F., R. Iorio, J. W. Burby, C. Liu and E. Hirvijoki. Dispersion relation for gauge-free electromagnetic drift kinetics. Submitted to *Physics of Plasmas*. (LA-UR-21-25075)

Reports

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Presentation Slides

Burby, J. W. Integrating guiding center motion in loop space. . (LA-UR-19-22767)

Burby, J. W. Compatibility Conditions for Quasisymmetry. . (LA-UR-19-27161)

Burby, J. W. Slow manifold integrators and the errors the commit. . (LA-UR-19-28965)

Burby, J. W. Slow manifold integrators: basic theory. Presented at *Nambe Meeting*, Los Alamos, New Mexico, United States, 2020-01-22 - 2020-01-22. (LA-UR-20-20600)

Burby, J. W. Slow manifold integrators: by way of computational Hamiltonian mechanics. Presented at *Structure-Preserving Geometric Discretization of Physical Systems*, Princeton, New Jersey, United States, 2020-02-17 - 2020-02-18. (LA-UR-20-21533)

Burby, J. W. Principles for implicit integration. . (LA-UR-21-25414)

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Burby, J. W., N. Kallinikos and R. MacKay. Grad-Shafranov equation for non-axisymmetric MHD equilibria. . (LA-UR-20-24872)

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Burby, J. W., Q. Tang and R. Maulik. Fast neural Poincare maps for toroidal magnetic fields. Presented at *SIAM Conference on Computational Science and Engineering*, Fort Worth, Texas, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-21970)

Burby, J. W. and Q. Tang. Fast neural Poincare maps for toroidal magnetic fields. . (LA-UR-20-24873)

Posters

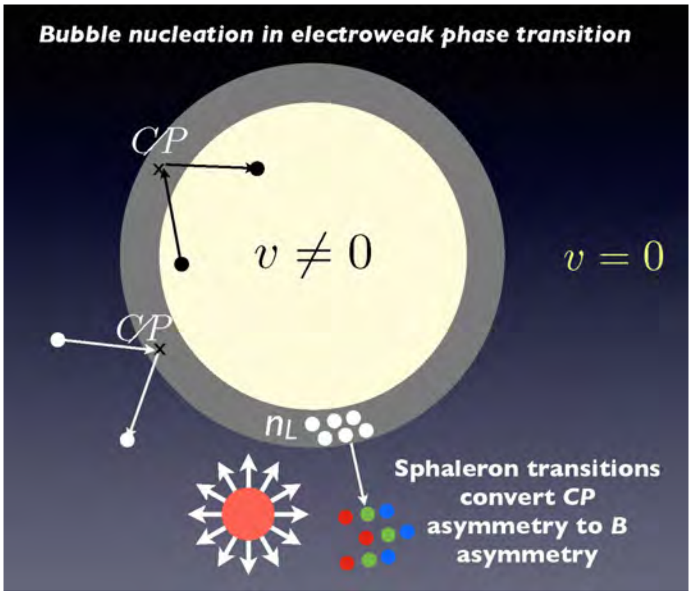
Burby, J. W. Slow manifold integrator for electromagnetic PIC. Presented at *2019 APS DPP meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30654)

**Peer-reviewed*

State-of-the-Art Predictions for the Matter-Antimatter Asymmetry

Christopher Lee

20190622PRD2



A fraction of a second after the Big Bang, the universe cools to a temperature when the Higgs field phase transitions from zero to a nonzero value (v) and nucleates bubbles where particles gain nonzero mass. Particles and antiparticles interact with the bubble walls with tiny differences, generating an asymmetry, which is converted by processes known as sphalerons into the baryon number that makes up the visible universe today. Los Alamos physicists use quantum field and transport theory to predict how much matter this mechanism can generate and how to test it with collider and precision neutron experiments today.

Project Description

This project addresses two of the great open scientific questions of our day, which are also two of the top research priorities of the Department of Energy Office of Science: "What is the origin of the matter-antimatter asymmetry?" and "What lies beyond the Standard Model of Particle Physics?" The first question addresses the origin of all visible matter in our universe today, which cannot be explained by the current Standard Model of Particle physics, thus connecting it to the second question. Answers to these require the development of frontier theoretical and computational tools as well as experimental techniques to probe physical phenomena lying beyond the Standard Model that could provide these answers. In addition, the theoretical tools are applicable to studying other physical systems, such as supernovae and how the propagation of neutrinos through them affects the dynamics of their explosions, while the experiments develop cutting-edge technology and capabilities in accelerator science and in trapping and measuring precisely ultracold neutrons. At the conclusion of our project, besides having such new tools and capabilities, we expect to have made a major step towards understanding how the matter in the universe could have been generated in its first few moments of existence.

Technical Outcomes

This project demonstrated, using new theoretical tools that were developed over its course, that a whole set of new measurements at upcoming experiments (such as colliders, muon and neutrino measurements, and neutron electric dipole moment searches) can probe and demonstrate whether certain models or scenarios of physics beyond the Standard Model might be realized in Nature and account for the amount of excess matter over antimatter in the current universe.

Publications

Journal Articles

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*F. K. *. L. C. *. M. E. *. Y. B. Cirigliano, V. *., V. Cirigliano, K. Fuyuto, C. Lee, E. Mereghetti and B. Yan. Charged lepton flavor violation at the EIC. 2021. *Journal of High Energy Physics*. **2021** (3): 256. (LA-UR-21-20531 DOI: 10.1007/JHEP03(2021)256)

*Cirigliano, V., K. Fuyuto, M. J. Ramsey-Musolf and E. Rule. Next-to-leading order scalar contributions to μ → e conversion. 2022. *Physical Review C*. **105** (5): 055504. (LA-UR-21-32420 DOI: 10.1103/PhysRevC.105.055504)

*Cirigliano, V., W. Dekens, J. de Vries, K. Fuyuto, E. Mereghetti and R. Ruiz. Leptonic anomalous magnetic moments in ν SMEFT. 2021. *Journal of High Energy Physics*. **2021** (8): 103. (LA-UR-21-24456 DOI: 10.1007/JHEP08(2021)103)

*Fuyuto, K., J. De Vries, P. Draper, J. Kozaczuk and B. Lillard. Uncovering an axion mechanism with the EDM portfolio. 2021. *Physical Review D*. **104** (5): 055039. (LA-UR-21-26248 DOI: 10.1103/PhysRevD.104.055039)

*Fuyuto, K., W. Hou and E. Senaha. Cancellation mechanism for the electron electric dipole moment connected with the baryon asymmetry of the Universe. 2020. *Physical Review D*. **101** (1): 011901. (LA-UR-19-30968 DOI: 10.1103/PhysRevD.101.011901)

*Mereghetti, E., K. Fuyuto, W. G. Dekens, J. de Vries and G. Zhou. Sterile neutrinos and neutrinoless double beta decay in effective field theory. 2020. *Journal of High Energy Physics*. **2020** (6): 97. (LA-UR-20-21376 DOI: 10.1007/JHEP06(2020)097)

Reports

Mereghetti, E., K. Fuyuto, B. Yan, S. Banerjee, V. Cirigliano, M. Dam, L. Fiorini, C. Gal, T. Husek, K. Monsalvez-Pozo, H. Peng, F. Polci, J. Portoles, A. Rostomyan, M. Villanueva, J. Zhang and X. Zhou. Charged lepton flavor violation in the tau sector. Unpublished report. (LA-UR-22-22663)

Presentation Slides

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Fuyuto, K. Search for lepton flavor violation at the EIC. Presented at *PPC 2021: XIV International Workshop on Interconnections between Particle Physics and Cosmology*, Norman, Oklahoma, United States, 2021-05-17 - 2021-05-17. (LA-UR-21-24724)

Fuyuto, K. Electroweak Baryogenesis in General Two Higgs Doublet Model. Presented at *Computations that Matter 2021*, Leiden, Netherlands, 2021-06-21 - 2021-06-21. (LA-UR-21-25750)

Fuyuto, K. Neutrinoless double beta decay with light sterile neutrinos. Presented at *A Virtual Tribute to Quark Confinement and the Hadron Spectrum 2021*, Virtual, Norway, 2021-08-02 - 2021-08-06. (LA-UR-21-27455)

Fuyuto, K. Fundamental symmetry tests in the lepton sector. . (LA-UR-21-31645)

Fuyuto, K. The Mystery of the Matter in the Universe. . (LA-UR-21-31644)

Fuyuto, K. Searches for violations of fundamental symmetries. . (LA-UR-22-20417)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-20967)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22082)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22446)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22469)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22561)

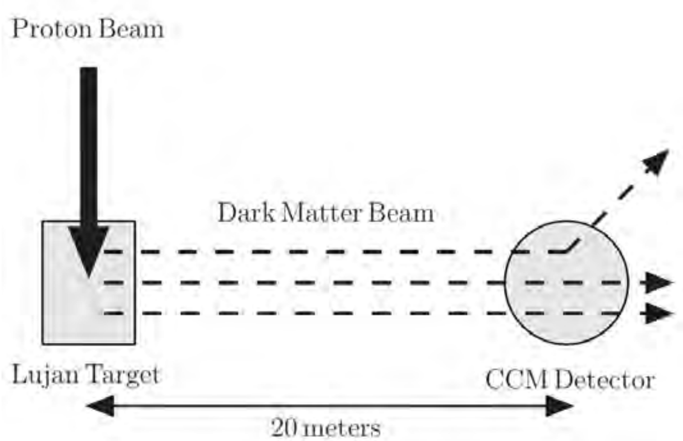
Fuyuto, K. Searching for new physics in CP violation. . (LA-UR-22-23320)

Fuyuto, K. Unraveling the origin of neutrino mass. . (LA-UR-22-28333)

**Peer-reviewed*

Searching for Dark Matter with Fixed Target Experiments

Daniele Spier Moreira Alves
20190626PRD2



Dark matter makes up most of the matter in the universe but has only been observed gravitationally despite numerous experimental efforts. This figure schematically describes a novel accelerator-based dark matter search possible at Los Alamos Neutron Science Center (LANSCE). The proton beam impacts the Lujan target, producing copious numbers of neutral pions. The neutral pions decay immediately and may very rarely produce dark matter particles. The produced dark matter radiates out from the target, reaching the Coherent CAPTAIN-Mills detector located 20 meters away and scattering coherently with the liquid argon inside. This project simulates the dark matter production and scattering process.

Project Description

The high level goal is explore the theory and interpretation of experimental data to discover the nature of dark matter in the Universe, an unknown form of matter in galaxies that is six times more abundant than ordinary matter. The expected outcome is a further understanding of the fundamental constituents of the Universe, either by discovering new forms of matter, of by ruling out existing theories that attempt to explain dark matter. This project addresses the challenges defined as high priority scientific goals by the Department of Energy Office of Science (DOE SC) Particle Physics Project Prioritization Panel (a subpanel of the High Energy Physics Advisory Panel), the 2015 Department of Energy Office of Science (SC) Nuclear Physics Long-Range Plan, and the Laboratory's Strategic Investment Plan, specifically in its Nuclear and Particle Futures pillar.

Technical Outcomes

This project redefined the state-of-the-art dark matter studies in proton beam fixed target experiments by producing a software simulation code for the calculation of dark matter signals. The model was adopted by experiments at Los Alamos and Oak Ridge National Laboratories, which produced the world’s best limits on light dark matter models. It is also used in the Snowmass process, a large study which will inform the decadal investment priorities of the Office of Science.

Publications

Journal Articles

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deNiverville, P., H. Lee and Y. Lee. New searches at the reactor experiments based on the dark axion portal. Submitted to *Physical Review D*. (LA-UR-21-20328)

deNiverville, P., L. Buonocore and C. Frugiuele. The hunt for sub-GeV dark matter at neutrino facilities: a survey of past and present experiments. Submitted to *Journal of High Energy Physics*. (LA-UR-19-32644)

Presentation Slides

deNiverville, P. Searching for Light Dark Matter with Fixed Target Neutrino Experiments. Presented at *T-2 Group Meeting*, Los Alamos, New Mexico, United States, 2021-01-21 - 2021-01-21. (LA-UR-21-20483)

deNiverville, P. MCNP Physics Model Comparison. Presented at *CCM Analysis Meeting*, Los Alamos, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-21358)

deNiverville, P. DM searches in neutrino beam experiments - near and far detectors. Presented at *Workshop on Interplay of Neutrino and Dark matter Experiments and Exotic Searches*, Suwon, Korea, South, 2021-03-18 - 2021-03-19. (LA-UR-21-22524)

deNiverville, P. Changes to Coherent Dark Matter Nucleus Scattering. Presented at *CCM Analysis Meeting*, Los Alamos, New Mexico, United States, 2021-04-29 - 2021-04-29. (LA-UR-21-24075)

deNiverville, P. Searching for Dark Matter with Neutrino Experiments. Presented at *T-Division Presentations*, Los Alamos, New Mexico, United States, 2021-06-16 - 2021-06-16. (LA-UR-21-25550)

**Peer-reviewed*

A Study of Diffusion Around Pulsar Wind Nebulae

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20200684PRD2

The High-Altitude Water Cherenkov (HAWC) Observatory is capable of observing cosmic gamma rays to energies trillions of times more energetic than visible light. Seen here, the HAWC array consists of 300 inner main detectors and 350 smaller "outrigger" detectors. By incorporating these outrigger detectors into the HAWC analysis chain, the HAWC sensitivity to the highest-energy galactic objects, such as pulsar-wind nebulae, will improve by more than a factor of 2. (Image Credit: HAWC Collaboration)

Project Description

Department of Energy (DOE), National Science Foundation (NSF), and National Aeronautics Space Administration (NASA) are all funding fundamental research to investigate the nature of dark matter. This project will result in the constraint of pulsar wind nebulae - one of the largest backgrounds in cosmic-ray dark matter searches. With these constraints, some dark matter models can be ruled out if no residual dark matter signal is detected. If positive signal is detected, then this enables experiments such as the High Altitude Water Cherenkov (HAWC) observatory to verify that such a signal is consistent with expected dark matter behavior. Discovery of dark matter would solve one of the longest standing problems in astrophysics, cosmology, and particle physics. These studies could also explain the unusually high density of cosmic electrons around the Earth and, potentially, will indicate the sources of the highest-energy cosmic particles in the Galaxy. The techniques used reduce trillions of events to only a few hundred high-energy gamma-rays and have broad applicability in other analyses around the Laboratory. This, along with searching for small signal in a noisy dataset and dealing with large datasets (over 4 petabytes of data) all are also extendable to the Lab's stockpile stewardship mission.

Technical Outcomes

The team created algorithms that relied on removing the noise from very large datasets and filtering out gamma rays. Two scientific studies were performed that quantified the behavior of pulsar wind nebulae in our Galaxy, which is an important background for dark matter searches. One study was a broad survey, while the other explored the gamma-ray emission of a single bright pulsar wind nebula in depth. The project was successful in achieving its goals.

Publications

Journal Articles

*Albert, A., R. Alfaro, C. Alvarez, J. D. Alvarez, J. R. Angeles Camacho, J. C. Arteaga-Velazquez, D. Avila Rojas, H. A. A. Solares, R. Babu, E. Belmont-Moreno, C. Brisbois, K. S. Caballero-Mora, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. C. de Leon, E. De la Fuente, C. de Leon, R. Diaz Hernandez, B. L. Dingus, M. A. DuVernois, M. Durocher, J. C. Diaz-Velez, K. Engel, C. Espinoza, K. L. Fan, K. Fang, M. Fernandez Alonso, N. Fraija, D. Garcia, J. A. Garcia-Gonzalez, F. Garfias, G. Giacinti, H. Goksu, M. M. Gonzalez, J. A. Goodman, J. P. Harding, J. Hinton, B. Hona, D. Huang, F. Hueyotl-Zahuantitla, P. Huntemeyer, A. Iriarte, A. Jardin-Blicq, V. Joshi, S. Kaufmann, D. Kieda, W. H. Lee, J. Lee, H. L. Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, K. Malone, V. Marandon, O. Martinez, J. Martinez-Castro, J. A. Matthews, P. Miranda-Romagnoli, J. A. Morales-Soto, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, M. U. Nisa, R. Noriega-Papaqui, L. Olivera-Nieto, N. Omodei, A. Peisker, Y. Perez Araujo, E. G. Perez-Perez, C. D. Rho, D. Rosa-Gonzalez, H. Salazar, F. Salesa Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, J. Serna-Franco, A. J. Smith, Y. Son, R. W. Springer, O. Tibolla, K. Tollefson, I. Torres, R. Torres-Escobedo, R. Turner, F. Urena-Mena, L. Villasenor, X. Wang, I. J. Watson, E. Willox, A. Zepeda, H. Zhou, M. Breuhaus, H. Li and H. Zhang. HAWC Study of the Ultra-high-energy Spectrum of MGRO J1908+06. 2022. *The Astrophysical Journal*. **928** (2): 116. (LA-UR-21-29999 DOI: 10.3847/1538-4357/ac56e5)

*Burgess, D. A., K. Mori, J. D. Gelfand, C. J. Hailey, Y. M. Tokayer, J. Woo, H. An, K. Malone, S. P. Reynolds, S. Safi-Harb and T. Temim. The Eel Pulsar Wind Nebula: A PeVatron-candidate Origin for HAWC J1826−128 and HESS J1826−130. 2022. *The Astrophysical Journal*. **930** (2): 148. (LA-UR-21-30784 DOI: 10.3847/1538-4357/ac650a)

Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-25495 DOI: 10.22323/1.395.0810)

Malone, K. A. A search for spectral hardening in HAWC sources above 56 TeV. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-25494 DOI: 10.22323/1.395.0811)

Malone, K. A., J. P. Harding, A. Albert, M. Durocher, S. Casanova, D. Huang, F. Salesa Greus, B. L. Dingus, G. J. Kunde, C. Brisbois and H. Zhou. Evidence of 200 TeV photons from HAWC J1825-134. Submitted to *Nature Astronomy*. (LA-UR-20-28703)

Malone, K. A., J. P. Harding, B. L. Dingus, M. Durocher, A. Albert, H. Zhou, C. Brisbois and V. Baghmanyan. Evidence that Ultra-High-Energy Gamma Rays are a Universal Feature Near Powerful Puslars. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-20344)

Malone, K. A. and B. L. Dingus. Multi-wavelength observations of 2HWC J1928+177: dark accelerator or new TeV gamma-ray binary?. Submitted to *Astrophysical Journal*. (LA-UR-20-28702)

Mori, K., H. An, K. A. Malone, C. Hailey, B. Humensky, B. L. Dingus, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR broad-band X-ray observational campaign of energetic pulsar wind nebulae in synergy with VERITAS, HAWC and Fermi gamma-ray telescopes. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-26689 DOI: 10.22323/1.395.0963)

Mori, K., H. An, K. A. Malone, C. Hailey, B. Humensky, B. L. Dingus, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR broad-band X-ray observational campaign of energetic pulsar wind nebulae in synergy with VERITAS, HAWC and Fermi gamma-ray telescopes. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-26689 DOI: 10.22323/1.395.0963)

Presentation Slides

Malone, K. A. Highest-energy gamma-ray emission from HAWC in the environments of powerful pulsars. Presented at *APS April Meeting*, Virtual, New Mexico, United States, 2020-04-18 - 2020-04-21. (LA-UR-20-22825)

Malone, K. A. HAWC results on other TeV halos. Presented at *1st Workshop on Gamma-ray Halos around Pulsars*, Rome (Virtual), Italy, 2020-12-01 - 2020-12-03. (LA-UR-20-29726)

Malone, K. A. Observation of the highest-energy gamma rays with the HAWC Observatory. Presented at *P-3 seminar*, Virtual, New Mexico, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-22661)

Malone, K. A. Observation of the highest-energy gamma rays with the HAWC Observatory. . (LA-UR-21-23951)

Malone, K. A. Recent results from the HAWC Observatory. Presented at *Seminar to be given to the Astroparticles and Cosmology Laboratory at the University of Paris next week*, Virtual, New Mexico, United States, 2021-05-05 - 2021-05-05. (LA-UR-21-24196)

Malone, K. A. Flash poster talk for "A search for spectral hardening in HAWC sources above 56 TeV". Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25496)

Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25532)

Malone, K. A. HAWC study of the ultra-high-energy gamma-ray source MGRO J1908+06. Presented at *APS April 2021*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-23172)

Malone, K. A. HAWC's view of the highest-energy gamma-ray sky. Presented at *19th Divisional Meeting of the High Energy Astrophysics Division of the American Astronomical*

Society, Pittsburgh, Pennsylvania, United States, 2022-03-13 - 2022-03-17. (LA-UR-22-21960)

Malone, K. A., K. Mori, B. L. Dingus, H. An, C. J. Hailey, B. Humensky, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR X-ray observation campaign of energetic pulsar wind nebulae. Presented at *International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-26302)

Malone, K. A., K. Mori, B. L. Dingus, H. An, C. J. Hailey, B. Humensky, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR X-ray observation campaign of energetic pulsar wind nebulae. Presented at *International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-26302)

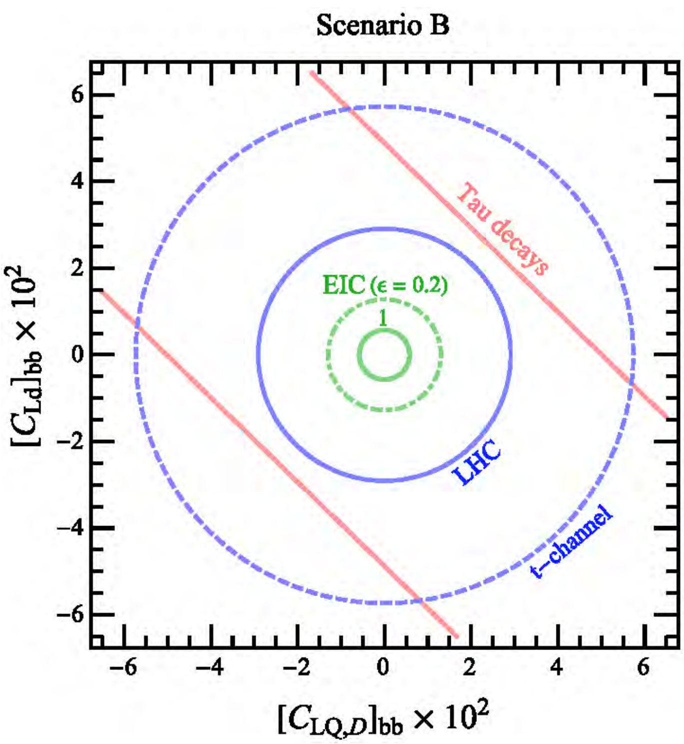
Posters

Malone, K. A. A search for spectral hardening in HAWC sources above 56 TeV. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25493)

**Peer-reviewed*

Searching for New Physics at the Intensity Frontier at the Electron-Ion Collider

Christopher Lee
20200775PRD4



LANL theoretical physicists' computations demonstrate that the upcoming Electron-Ion Collider (EIC) may have several times greater sensitivity (green lines) than competing measurements at the Large Hadron Collider (LHC) (blue lines) or tau lepton decay measurements (red lines) to charged lepton flavor violating new physics phenomena that change lepton flavor (e.g. electron to tau) in scatterings of electrons from heavy virtual bottom (b) quarks in the proton, an exciting new physics thrust for the EIC.

Project Description

This project will advance our ability to discover new elementary particles and forces with high-energy particle colliders, especially the upcoming Electron-Ion Collider (EIC), which will place the United States (US) at the forefront of worldwide high-energy electron-proton collider technology. We will perform the theoretical calculations, using the most modern tools in quantum field theory, to predict and optimize the sensitivity of the EIC to new physics interactions that may violate "charged lepton flavor conservation", leading to phenomena like electrons re-emerging in these collisions as heavier leptons like muons or tau leptons. Discovering and characterizing the origin of such new interactions would shed light on some of the most pressing and puzzling problems in fundamental physics today, such as where neutrino masses come from or how the excess of matter over antimatter in our universe originated. Our work will result in better guidance for detector design and optimization at EIC to find charged lepton flavor changing events, and optimize the strategies to analyze data to discover and characterize the underlying origin of such new phenomena. It will contribute to the worldwide impact of the US nuclear physics effort in collider physics.

Technical Outcomes

This project led to a comprehensive study of the sensitivity of the future Electron-Ion Collider to new physics beyond the Standard Model that involves interactions that violate conservation of charged lepton flavor. Such new physics could be responsible for neutrino masses and mixings and the origin of matter in the universe. The project also produced several papers proposing probes of new physics in several types of colliders.

Publications

Journal Articles

*F. K. *. L. C. *. M. E. *. Y. B. Cirigliano, V. *., V. Cirigliano, K. Fuyuto, C. Lee, E. Mereghetti and B. Yan. Charged lepton flavor violation at the EIC. 2021. *Journal of High Energy Physics*. **2021** (3): 256. (LA-UR-21-20531 DOI: 10.1007/JHEP03(2021)256)

*Dong, H., P. Sun, B. Yan and C. -. Yuan. Probing the Zbb\xc2\xaf anomalous couplings via exclusive Z boson decay. 2022. *Physics Letters B*. **829**: 137076. (LA-UR-22-20027 DOI: 10.1016/j.physletb.2022.137076)

Li, H. T., B. Yan and C. P. Yuan. Jet Charge: A new tool to probe the anomalous Zbb couplings at the HERA and EIC. Submitted to *PLB*. (LA-UR-21-31134)

*Liu, Y., B. Yan and R. Zhang. Loop induced top quark FCNC through top quark and dark matter interactions. 2022. *Physics Letters B*. **827**: 136964. (LA-UR-21-22425 DOI: 10.1016/j.physletb.2022.136964)

Liu, y. and B. Yan. Searching for the axion-like particle at the EIC. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-21-31766)

*Yan, B. Determining Higgs boson width at electron-positron colliders. 2021. *Physics Letters B*. **822**: 136709. (LA-UR-21-24315 DOI: 10.1016/j.physletb.2021.136709)

Yan, B. Probing the dark photon via polarized DIS scattering at the HERA and EIC. 2022. *Physics Letters B*. **833**: 137384. (LA-UR-22-21939 DOI: 10.1016/j.physletb.2022.137384)

*Y. Z. *. Y. C. Yan, B. *. and B. Yan. The anomalous Zbb couplings at the HERA and EIC. 2021. *Physics Letters B*. **822**: 136697. (LA-UR-21-26072 DOI: 10.1016/j.physletb.2021.136697)

*Yan, B. and C. P. Yuan. Anomalous Zbb Couplings: From LEP to LHC. 2021. *Physical Review Letters*. **127** (5): 51801. (LA-UR-21-20373 DOI: 10.1103/PhysRevLett.127.051801)

*Yan, B. and K. Xie. Probing the electroweak symmetry breaking with Higgs production at the LHC. 2021. *Physics Letters B*. **820**: 136515. (LA-UR-21-24074 DOI: 10.1016/j.physletb.2021.136515)

Reports

Mereghetti, E., K. Fuyuto, B. Yan, S. Banerjee, V. Cirigliano, M. Dam, L. Fiorini, C. Gal, T. Husek, K. Monsalvez-Pozo, H. Peng, F. Polci, J. Portoles, A. Rostomyan, M. Villanueva, J. Zhang and X. Zhou. Charged lepton flavor violation in the tau sector. Unpublished report. (LA-UR-22-22663)

Presentation Slides

Lee, C., B. Yan, B. Yoon, G. Bell, Y. Makris and J. Talbert. Angularities, gaps, and \\alpha_s. Presented at *World SCET 2021*, Cambridge, Massachusetts, United States, 2021-04-19 - 2021-04-23. (LA-UR-21-23742)

Lee, C., B. Yoon, B. Yan, Y. Makris, J. Talbert and G. Bell. Event shape tails and alpha_s. Presented at *INT Workshop on Probing QCD at High Energy and Density with Jets*, Seattle, Washington, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-27921)

Lee, C., E. Mereghetti and B. Yan. Searching for New Physics at the Intensity Frontier at the EIC: Project Visit. . (LA-UR-21-29821)

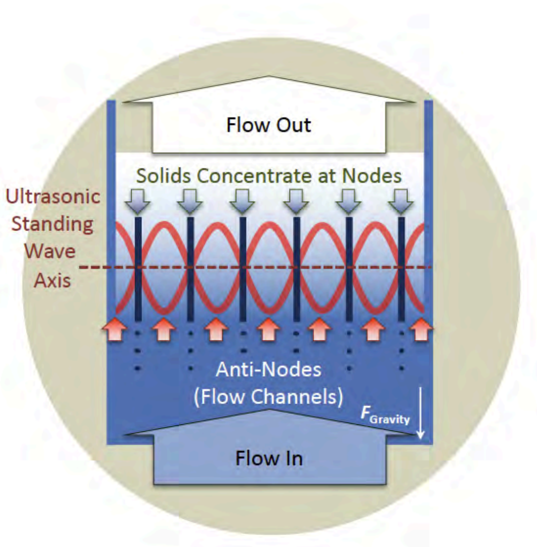
Yan, B. From Precision calculation to new physics searches at colliders. . (LA-UR-21-22158)

Yan, B., C. Lee, V. Cirigliano, K. Fuyuto and E. Mereghetti. Searching for Charged Lepton Flavor Violation at the EIC. Presented at *IAS Program on High Energy Physics 2021*, Hong-Kong, China, 2021-01-14 - 2021-01-21. (LA-UR-21-20485)

**Peer-reviewed*

Implementing a Novel Ultrasonic Filtration Technology to Eliminate Hydroxide Precipitation Bottlenecks at Technical Area (TA)-55

James Coons
20210538MFR



Removing hydroxide precipitates with vacuum filtration is a slow, time consuming process that poses risks to glovebox workers and generates waste membranes. Ultrasonic filtration is a membrane-free technology that traps particles in a standing wave while creating wide channels that allow the clarified liquid to pass through unhindered. Large aggregates are formed that settle quickly against the incoming flow and accumulate in the bottom of the chamber for steady removal. Ultrasonic filtration is being automated to eliminate process bottlenecks at TA-55 and reduce the overall footprint of hydroxide precipitate processing.

Project Description

The ultimate goal of this endeavor is a functional revolutionary hydroxide precipitation process which utilizes a novel separation technology called ultrasonic filtration. This disruptive technology would replace a physical membrane with an ultrasonic field that retains solid particles while allowing the particle-free media to pass through. By eliminating the physical barrier, solids removal occurs much faster in a closed, continuous operation. Ultrasonic filtration will eliminate the separation bottle necks at Technical Area-55 of Los Alamos National Laboratory, dramatically reduce dose and physical demands on operators, and improve the caustic glovebox atmospheres that contribute to equipment corrosion and limited lifetimes. This groundbreaking hydroxide precipitation process builds upon existing ultrasonic separations technology, but substantial work is required to produce a functional system in a flow-through configuration operational in gloveboxes in nuclear facilities. This Phase 1 project aims to understand performance-bounding properties including the settling behavior of surrogate hydroxide particles and aggregates, and assess the performance of ultrasonic filtration over a range of scales. These baseline tests are essential for the Phase 2 study focusing on overcoming fundamental impediments for improved prototype system performance.

Technical Outcomes

The project advanced understanding of hydroxide precipitates and their dewatering challenges. Vicinal water presents a formidable barrier to hydroxide precipitate dewatering. High or complete particle removal is attainable by implementing rapid (≥ 1 liter per hour) ultrasonic filtration for bulk water removal and removal of vicinal water by heating or enhanced evaporation. The team observed an optimum hydrogen (pH) range of between 9 and 11 for Cerium/Zirconium (Ce/Zr) precipitates, based on settling velocities and/or solubility considerations.

Publications

Presentation Slides

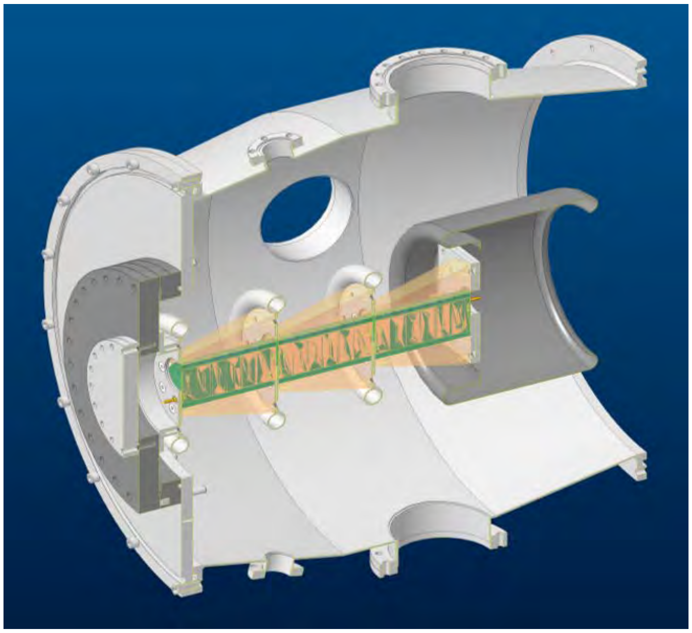
Roman, A. R., J. E. Coons and A. J. Parkison. Ultrasonic Filtration: A Revolutionary Technology for Hydroxide Precipitation. Presented at *Engineering Week Webex Meeting*, Los Alamos, New Mexico, United States, 2021-02-22 - 2021-02-24. (LA-UR-21-21714)

Roman, A. R. and J. E. Coons. Ultrasonic Separation of Hydroxide Precipitates. Presented at *Actinide Separations Conference*, Los Alamos, New Mexico, United States, 2022-05-18 - 2022-05-19. (LA-UR-22-24651)

**Peer-reviewed*

Megavolt Generator for Multiple-Pulse Hydrotesting

Nicola Winch
20210540MFR



Los Alamos leads the world in multiple-pulse radiography but this can only be done at very large accelerator facilities such as DARHT and LANSCE. PHOENIX is a portable, high-energy, multiple-pulse radiographic source which can return multiple-pulse radiography to the small scale firing sites.

Project Description

Los Alamos leads the world in multiple-pulse radiography but this can only be done at very large accelerator facilities such as the Dual-Axis Radiographic Hydrodynamic Test (DARHT) Facility and Los Alamos Neutron Science Center (LANSCE). This is very expensive, and a lot of types of shots would benefit from smaller scale, low cost, portable, multiple pulse radiography. PHOENIX (Portable, High efficiency, Optimal ENergy, Imaging X-rays) can return multiple-pulse radiography to the small scale firing sites. Current x-ray generators at small scale firing sites are 1960s Febetrons, which have both safety and reliability issues and are not multiple pulsed machines. PHOENIX will benefit the weapons engineering mission by providing portable multiple pulse radiography to the small scale firing sites, a Los Alamos Goal since the Manhattan Project. A modified version would benefit the global security mission by providing a man portable, low power, megavolt source to nuclear emergency response teams.

Technical Outcomes

This project successfully demonstrated a multiple pulsed x-ray source with a maximum endpoint energy of 600 kilovolt. The highest energy radiograph ever taken with a source capable of running on battery power. Multiple-pulsing was demonstrated with both an explosive-bridge-wire, plasma-cathode and a two-pulse cathode circuit. Pulse width and spacing was controlled with compact, solid-state circuits rather than much larger, conventional pulsed-power. Designs for the next generation systems were made.

Publications

Presentation Slides

Misurek, L. A., J. D. Goettee, D. Platts, C. D. Romero, E. B. Sorensen, S. A. Watson and N. M. Winch. PHOENIX Megavolt X-ray Source. Presented at *J32HDT RSIA meeting*, Las Vegas, Nevada, United States, 2023-03-21 - 2023-03-23. (LA-CP-23-20178)

Posters

Misurek, L. A., S. A. Watson, N. M. Winch, E. B. Sorensen and D. Platts. PHOENIX Megavolt Radiography Source. Presented at *WORIA Radiography Conference*, Oak Ridge, Tennessee, United States, 2023-02-07 - 2023-02-09. (LA-UR-23-20629)

**Peer-reviewed*

Cryogenic Wakefield Absorbers for C-Band Accelerators

Evgenya Simakov
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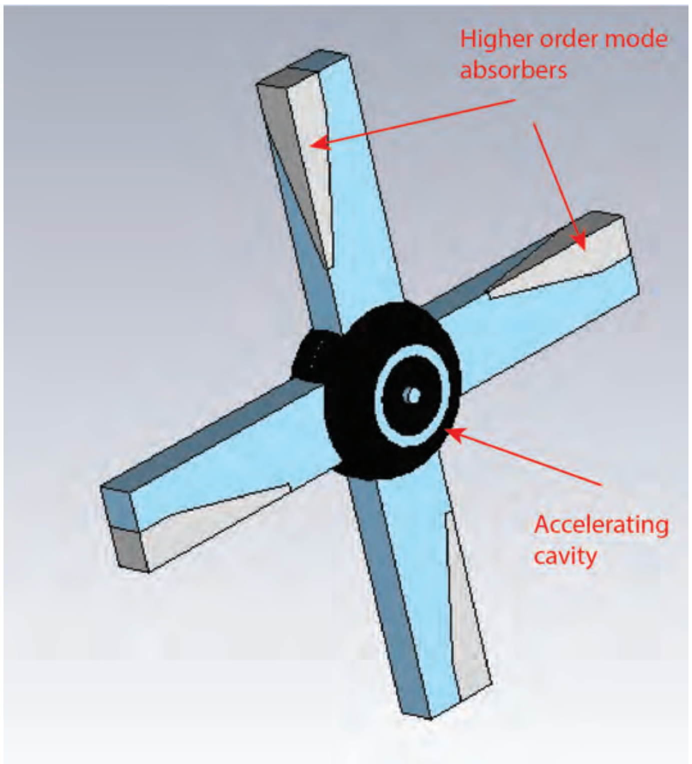

This project will test various absorbing materials for suppressing higher order modes in cryogenically-cooled accelerators, identifying the material with the best absorbing properties at the temperature of 40 Kelvin. The materials will act in higher order mode absorbers placed at the periphery of an accelerating cavity to suppress higher order mode wakefields, that are parasitic cavity modes generated during particle beam acceleration.

Project Description

Particle accelerators are established tools for solving national security challenges, as well as for discovery science. Current missions with national security implications include the need to study and develop materials under extreme conditions that never have been accessible before, higher energy accelerators for proton radiography for stockpile stewardship, and improved tools for remote sensing in defense from national security threats. These represent the range of accelerator systems from large to small. The tools and technologies developed in this project will enable follow-on technology development efforts with significant impact on the performance and cost of accelerator systems. Novel design and engineering tools will provide the first ever integrated radio-frequency (RF)-structure design that will operate in a cryogenic environment of 40 Kelvin with reduced parasitic higher order modes.

Technical Outcomes

The project developed a testing assembly to study dielectric and magnetic properties of lossy materials between 5 and 20 gigahertz. The materials were cooled to a cryogenic temperature of 7 Kelvin. Data was collected during the warm-up. The team found that lossy properties of aluminum nitride ceramics (AIN) were almost independent of the temperature. The project concluded that AlN ceramics are suitable for fabricating higher order mode absorbers for cryo-cooled normal conducting high-gradient accelerating structures.

Publications

Journal Articles

S. Cerezo de la Roca, M. V., D. Garcia-Martin and M. Larocca. Effects of quantum noise on the overparametrization of quantum neural networks. Submitted to *Quantum Machine Intelligence*. (LA-UR-22-33019)

S. Cerezo de la Roca, M. V., L. Schatzki, M. Larocca and F. A. Sauvage. Theoretical Guarantees for Sn-Equivariant Quantum Neural Networks. Submitted to *Nature Communications*. (LA-UR-22-29899)

S. Cerezo de la Roca, M. V., M. Ragone, P. Braccia, Q. T. Nguyen, L. Schatzki, P. J. Coles, F. A. Sauvage and M. Larocca. Representation Theory for Geometric Quantum Machine Learning. Submitted to *Quantum*. (LA-UR-22-30670)

S. Cerezo de la Roca, M. V., Q. T. Nguyen, L. Schatzki, P. Braccia, M. Ragone, P. J. Coles, F. A. Sauvage and M. Larocca. Theory for Equivariant Quantum Neural Networks. Submitted to *Physical Review X*. (LA-UR-22-30859)

Sauvage, F. A., M. Larocca, P. J. Coles and M. V. S. Cerezo de la Roca. Building spatial symmetries into parameterized quantum circuits for faster training. Submitted to *Quantum*. (LA-UR-22-27391)

Conference Papers

Simakov, E. I., D. V. Gorelov, M. E. Middendorf, T. Tajima, M. R. A. Zuboraj and S. G. Biedron. C-BAND HIGH GRADIENT TESTING OF THE BENCHMARK a/\xce\xbb=0.105 CAVITY. Presented at *13th International Particle Accelerator Conference IPAC2022*. (Bangkok, Thailand, 2022-06-12 - 2022-06-12). (LA-UR-22-25323)

Presentation Slides

Sauvage, F. A., M. Larocca, P. J. Coles and M. V. S. Cerezo de la Roca. Building spatial symmetries into parameterized quantum circuits for faster training. Presented at *SQUINT 24th edition*, Berkeley, California, United States, 2022-10-20 - 2022-10-22. (LA-UR-22-30936)

Sauvage, F. A., M. Larocca, P. J. Coles and M. V. S. Cerezo de la Roca. Building spatial symmetries into parameterized quantum circuits for faster training. Presented at *Quantum Techniques in Machine Learning (QTML)*, Naples, Italy, 2022-11-07 - 2022-11-12. (LA-UR-22-31694)

**Peer-reviewed*

Novel Method of Manufacturing of the Conventional-Band Radiofrequency (RF) Cavity

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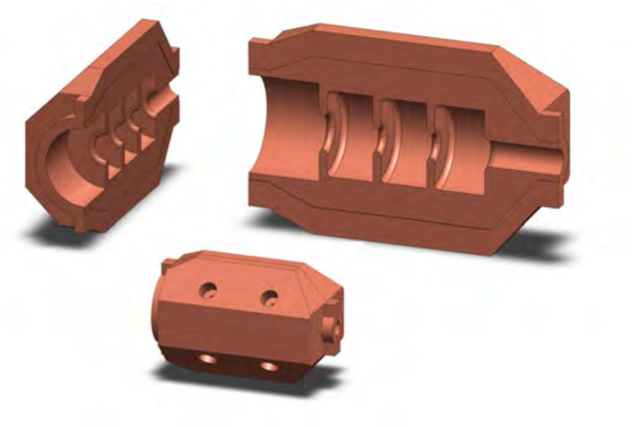
20220502MFR



Conventional-band (C-band) test RF cavity (design is developed at LANL in collaboration with the Stanford Linear Accelerator Center (SLAC) and the University of California, Los Angeles) is a testbed to understand the breakdown process during the high-power RF pulse. Making the cavity able to be re-assembled after opening and inspection would significantly increase the pace of developing new and perspective RF accelerating structures.

Project Description

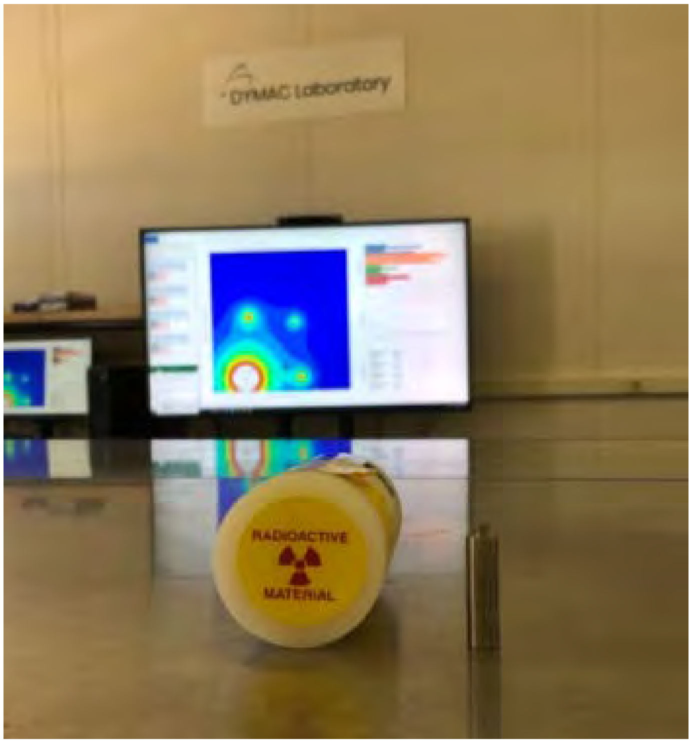
Accelerator technology is acknowledged as an enabling Los Alamos National Laboratory (LANL) capability for a broad range of National Security missions. This project will have a direct impact on the plans for modernization and upgrades to the high energy sections of Los Alamos Neutron Science Center (LANSCE) at moderate cost. Use of high gradient copper cavities will reduce the cost of the proposed LANSCE upgrades toward 3 giga-electron volt (GeV) or higher for proton radiography (pRad) by providing possibility to construct a high gradient booster that can fit into existing tunnel and experimental areas (like LANSCE). The new technology also has a direct path to being adapted for the construction of an electron accelerator planned for the Dynamic Mesoscale Material Science Capability (DMMSC) / Matter-Radiation Interactions in Extremes (MaRIE) project with the very similar benefits of reducing the footprint and construction cost as compared to the accelerator design that uses Superconducting radio frequency accelerating structures. Also, the project may benefit some of the Global Security programs that have interest in compact accelerators such as the remote Special Nuclear Materials (SNM) detection and accelerator applications in space.

Technical Outcomes

This project successfully developed and tested a mechanical prototype permitting multiple radio-frequency cavity disassembly and re-assembly. The reliable cavity re-assembly mechanism permits the examination of inner cavity surface modifications, including detailed observation of precursor formation that lead towards formation of the discharge sites. The project resulted in two designs.

Nuclear Material Control and Accounting (NMC&A)/In-line Monitoring Capability (ILM)

Rollin Lakis
20200668DI



Deployed in a simulated glovebox environment, a new sparse neutron and gamma ray detector array is used to measure and locate unknown radioactive materials. New approaches in near real time nuclear material situational awareness are being explored at Los Alamos. The Director's Initiative work explores the frontiers of domestic and international safeguards implementation to improve nuclear material accounting and safety in complex nuclear production environments.

Project Description

The primary goal of the In-Line Monitoring Project is to enhance manufacturing agility and efficiency in a nuclear material production environment, and improve nuclear security by modernizing, streamlining and optimizing quantitative nuclear material measurements and nuclear material control and accounting (NMC&A). Increased confidence will be achieved through the use of modern data analysis and statistical approaches coupled with optimized nondestructive assay (NDA) instruments, applied in-line or at-line in nuclear production environments.

Technical Outcomes

The project team constructed of mock-up glovebox line with neutron detector networks for real-time dynamic background monitoring. The team developed algorithms for dynamic background correction in real time. The project adapted Design of Experiments framework for Nuclear Material Control and Accountability to optimize Key Measurement Point selection and instrumentation. The team developed source localization algorithms for enhanced situational awareness and Nuclear Material Control, and developed and tested several Digital Twin related to the testbed.

Publications

Journal Articles

Skurikhin, A. N., T. J. I. Stockman, B. P. Weaver, S. E. Sarnoski, R. E. Lakis and V. Henzl. Wavelet-based Detection of Nuclear Material Movement. Submitted to *Journal of Nuclear Materials Management*. (LA-UR-22-30161)

Conference Papers

Ren, C. X., E. M. Casleton, S. E. Sarnoski, T. J. I. Stockman, A. N. Skurikhin, B. P. Weaver, V. Henzl, A. Favalli and R. E. Lakis. Source term estimation via combined sparse convex optimization and maximum liklihood extimation for nuclear material accounting. Presented at *INMM*. (Virtual, Austria, 2021-08-23 - 2021-09-01). (LA-UR-21-27798)

Sarnoski, S. E., M. A. Root and A. B. Iyer. Analysis of Dosimetry Capabilities Using Optically Stimulated Luminescence Fibers. Presented at *INMM 63rd Annual Meeting*. (Virtual, New Mexico, United States, 2022-07-24 - 2022-07-28). (LA-UR-22-26032)

Sarnoski, S. E., T. J. I. Stockman, E. M. Casleton, C. W. Graham, V. Henzl, M. Iliev, P. M. Mendoza, M. R. Newell, C. D. Rael, C. X. Ren, A. N. Skurikhin, J. Stinnett, D. T. Vo, B. P. Weaver, R. Weinmann-Smith, A. Favalli and R. E. Lakis. Analysis of in-line plutonium mass measurements, in a dynamic background environment, for nuclear material control and accounting in nuclear fuel cycle facilities. Presented at *INMM 2021 Annual Meeting*. (Virtual, New Mexico, United States, 2021-08-23 - 2021-08-26). (LA-UR-21-27969)

Presentation Slides

Cattaneo, A., E. M. Casleton, C. Chavez, H. H. Erpenbeck, A. Favalli, W. H. Geist, V. Henzl, D. C. Henzlova, M. Iliev, K. E. Koehler, R. E. Lakis, P. M. Mendoza, M. R. Newell, C. D. Rael, C. X. Ren, S. E. Sarnoski, A. N. Skurikhin, J. Stinnett, T. J. I. Stockman, D. T. Vo, B. P. Weaver and R. Weinmann-Smith. DYMAC LDRD Review. . (LA-UR-21-25652)

DeGuire, T. G., D. M. South, O. G. Pannucci, T. J. I. Stockman, R. E. Lakis and S. E. Sarnoski. An Integrated Approach to Precision Neutron Measurements in a Dynamic Environment. . (LA-UR-22-28432)

Henzl, V., K. E. Koehler, P. M. Mendoza, S. E. Sarnoski and B. P. Weaver. Key Measurement Points Optimization. Presented at *INMM/ESARDA 2021*, Vienna, Austria, 2021-08-23 - 2021-08-23. (LA-UR-21-28602)

Hitson, S. C., V. Henzl, K. E. Koehler, P. M. Mendoza and S. E. Sarnoski. Key Measurement Points Optimization Project. Presented at *LANL Annual Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27495)

Lakis, R. E. In Line Monitoring / Dynamic Material Control (DYMAC): Advanced Non Destructive Analysis (NDA) and Real-Time Special Nuclear Materials (SNM) Inventory. . (LA-UR-21-28431)

Ren, C. X., E. M. Casleton, S. E. Sarnoski, T. J. I. Stockman, A. N. Skurikhin, B. P. Weaver, V. Henzl, A. Favalli and R. E. Lakis. Source term estimation via combined sparse convex optimization and maximum likelihood estimation for nuclear material accounting. Presented at *INMM*, Vienna, Austria, 2021-08-23 - 2021-08-23. (LA-UR-21-28019)

South, D. M., O. G. Pannucci, T. G. DeGuire, T. J. I. Stockman, S. E. Sarnoski and R. E. Lakis. Modeling of a High-Level Neutron Coincidence Counter in a Dynamic Environment. Presented at *Keepin Lightning Talks*, Los Alamos, New Mexico, United States, 2022-08-10 - 2022-08-10. (LA-UR-22-28365)

I. Stockman, T. J. Facility scale in-situ source localization and assay via a sparse 3He neutron detector array: enhancing nuclear material control and accounting in nuclear fuel cycle facilities. Presented at *INMM 2021*, Virtual, Austria, 2021-08-23 - 2021-08-25. (LA-UR-21-28490)

I. Stockman, T. J. Dynamic Material Control: Domestic tech with safeguards potential. Presented at *PONI Summer Conference*, Albuquerque, New Mexico, United States, 2022-09-07 - 2022-09-08. (LA-UR-22-29251)

Posters

DeGuire, T. G., D. M. South, O. G. Pannucci, T. J. I. Stockman, S. E. Sarnoski and R. E. Lakis. An Integrated Approach to Precision Neutron Measurements in a Dynamic Environment. Presented at *LANL summer student symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27532)

Pannucci, O. G., T. G. DeGuire, D. M. South, T. J. I. Stockman and R. E. Lakis. Algorithm for Mass Prediction of a Nuclear Source in a Dynamic Environment. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27508)

Sarnoski, S. E. and T. J. I. Stockman. Analysis of in-line plutonium mass measurements, in a dynamic background environment, for nuclear material control and accounting in nuclear fuel cycle facilities. Presented at *INMM Annual Meeting*, Virtual, New Mexico, United States, 2021-08-23 - 2021-08-23. (LA-UR-21-28134)

South, D. M., O. G. Pannucci, T. G. DeGuire, T. J. I. Stockman, S. E. Sarnoski and R. E. Lakis. Digital Twin of a High--Level Neutron Coincidence Counter in a Dynamic Environment. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27551)

**Peer-reviewed*

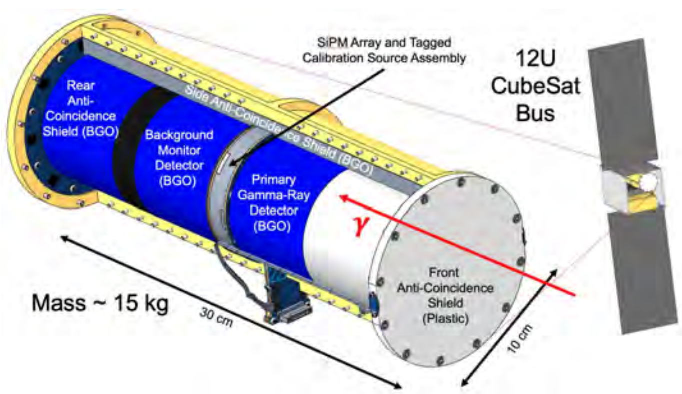
Science of Signatures

Science of Signatures

Directed Research
Continuing Project

The Mini Astrophysical Mega Electron-volt Background Observatory (MAMBO) CubeSat Mission: Demonstrating Agile Satellite Platforms for Astrophysics and National Security

Peter Bloser
20210047DR



High-quality gamma-ray measurements in space are technically challenging due to the intense radiation fields that exist above the atmosphere. The Mini Astrophysical MeV Background Observatory (MAMBO) mission will demonstrate a new approach to detecting gamma rays in space by flying an innovative detector on a "CubeSat," a satellite no bigger than a microwave oven and weighing less than 50 pounds. MAMBO achieves high efficiency and exceptional background rejection using an novel shielding configuration, pictured here. Using this approach, MAMBO will make the best-ever measurement of the mysterious, faint gamma-ray glow emanating from the distant Universe.

Project Description

Gamma-ray sensing from space is a critical capability for the Nation's national security and scientific missions. Though vital for both the detection of exo-atmospheric nuclear detonations and the study of energetic astrophysical phenomena, high-quality gamma-ray measurements in space are technically challenging due to the intense radiation fields that exist above the atmosphere. The entire spacecraft is bombarded by high-energy particles from deep space and the Sun, causing it to glow so brightly in gamma-rays that weak signals of interest are often obscured. The Mini Astrophysical MeV Background Observatory (MAMBO) mission will demonstrate a new approach to detecting gamma rays in space by flying an innovative detector on a "CubeSat," a satellite no bigger than a microwave oven and weighing less than 50 pounds. Such a small spacecraft will glow much less brightly. We will validate this approach via a challenging astronomical observation: the best-ever measurement of the mysterious, faint gamma-ray "background" emanating from the distant Universe. MAMBO will thus provide an important scientific result while demonstrating a new, flexible paradigm for space-based sensing for national security missions such as the National Nuclear Security Administration's space-based nuclear detonation detection (SNDD) program.

Publications

Journal Articles

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Bloser, P. F., W. Thomas Vestrand, M. P. Hehlen, L. P. Parker and A. S. Hoover. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat mission. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-29829 DOI: 10.1117/12.2576143)

Conference Papers

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel, R. H. Scobie, A. E. Nelson, T. J. Roth and D. C. Poulson. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat mission for gamma-ray astronomy. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Montreal, Canada, 2022-07-17 - 2022-07-22). (LA-UR-22-26134)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker, D. T. Beckman, J. M. McGlown, L. Holguin, K. K. Katko, J. D. Sedillo, A. E. Nelson and G. K. Lee. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *35th Annual Small Satellite Conference*. (Online, New Mexico, United States, 2021-08-07 - 2021-08-12). (LA-UR-21-25162)

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Reports

Fryer, C. L. MAMBO Institutional Computing Progress Report. Unpublished report. (LA-UR-22-20974)

Hehlen, M. P. and K. K. Katko. Formal Request for Information (RFI): Ground Stations for LANL CubeSats. Unpublished report. (LA-UR-21-26278)

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Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, L. Holguin, J. M. Michel, A. E. Nelson and D. C. Poulson. Let's MAMBO (Mini Astrophysical MeV Background Observatory)! A New CubeSat Mission at Los Alamos National Laboratory. Presented at *The 37th Annual New Mexico Symposium*, Online, New Mexico, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31383)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. M. McGlown, J. D. Sedillo, J. M. Michel, R. H. Scobie, A. E. Nelson, T. J. Roth and D. C. Poulson. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission for Gamma-Ray Astronomy. Presented at *SPIE Astronomical Telescope + Instrumentation*, Montreal, Canada, 2022-07-17 - 2022-07-22. (LA-UR-22-26886)

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Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker and A. S. Hoover. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *SPIE Astronomical Telescopes + Instrumentation*, Online, New Mexico, United States, 2020-12-13 - 2020-12-18. (LA-UR-20-29730)

Bloser, P. F. and M. P. Hehlen. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *Small Satellite Conference*, Logan, Utah, United States, 2022-08-08 - 2022-08-12. (LA-UR-22-27421)

Hehlen, M. P. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *SmallSat 2022*, Logan, Utah, United States, 2022-08-07 - 2022-08-11. (LA-UR-22-27554)

Posters

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel, R. H. Scobie, A. E. Nelson, D. C. Poulson, T. J. Roth, C. L. Fryer, A. L. Hungerford and M. R. Mumpower. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *19th Divisional Meeting of the High Energy Astrophysics Division*, Pittsburgh, Pennsylvania, United States, 2022-03-13 - 2022-03-17. (LA-UR-22-22176)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel, R. H. Scobie, A. E. Nelson, D. C. Poulson, T. J. Roth, C. L. Fryer, A. L. Hungerford, M. R. Mumpower, M. A. Rasmussen, S. Anandagoda, M. Ajello and D. Hartmann. The Mini Astrophysical MeV Background Observatory (MAMBO): A

CubeSat Mission for Gamma-Ray Astronomy. Presented at *38th New Mexico Symposium*, Socorro, New Mexico, United States, 2023-02-17 - 2023-02-17. (LA-UR-23-21435)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel, R. H. Scobie, A. E. Nelson, D. C. Poulson, T. J. Roth, C. L. Fryer, A. L. Hungerford, M. R. Mumpower, M. A. Rasmussen, S. Anandagoda, M. Ajello and D. Hartmann. The Mini Astrophysical MeV Background Observatory (MAMBO): A CubeSat Mission for Gamma-Ray Astronomy. Presented at *AGN Santa Fe: Where are the Objects in AGN Disks?*, Santa Fe, New Mexico, United States, 2023-03-22 - 2023-03-24. (LA-UR-23-22704)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel, R. H. Scobie, A. E. Nelson, D. C. Poulson, T. J. Roth, C. L. Fryer, A. L. Hungerford, M. R. Mumpower, M. A. Rasmussen, S. Anandagoda, M. Ajello and D. Hartmann. The Mini Astrophysical MeV Background Observatory (MAMBO): A CubeSat Mission for Gamma-Ray Astronomy. Presented at *20th HEAD Meeting*, WAIK\xc5\x8cLOA, Hawaii, United States, 2023-03-26 - 2023-03-30. (LA-UR-23-22836)

Poulson, D. C., P. F. Bloser, W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel, R. H. Scobie, A. E. Nelson, T. J. Roth, C. L. Fryer, A. L. Hungerford and M. R. Mumpower. Update on the Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *IEEE Nuclear Science Symposium and Medical Imaging Conference*, Milan, Italy, 2022-11-07 - 2022-11-12. (LA-UR-22-31540)

**Peer-reviewed*

HEROS- Human Exposure of Radiation using Organ Systems

Jennifer Harris
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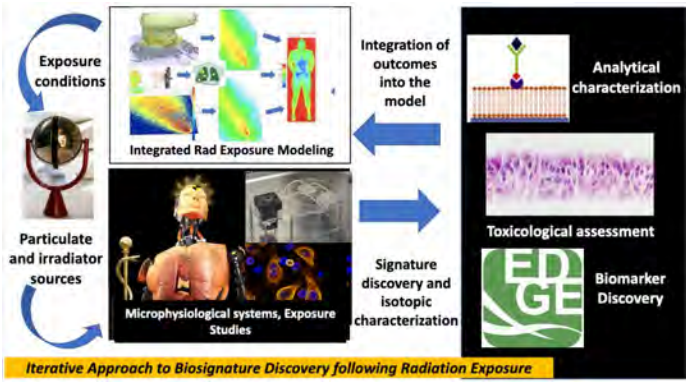

The Human Exposure of Radiation of Organ Systems (HEROS) project represents a suite of tools combined for the first time ever to systematically assess and discover biomarkers of low dose radiation exposure to laboratory-cultured microphysiological human organ systems. Modeling tools are being coupled to calculate dose from an event scenario to a specific organ tissue, fallout simulants and ionizing radiation are applied to laboratory organs, and both untargeted and targeted signature discovery is performed. Outcomes will be used to improve current models and human dose estimation tools.

Project Description

We will develop an integrated system for biosignature discovery, comprehensive assessment, empirical measurement and evaluation of radiation exposure on human beings by combining three novel technology portfolios: organs on a chip, theoretical modeling and empirical rad-bio measurements. Individual milestone scientific innovations include: 1) development of a first-of-its-kind integrated modeling system to compute organ-specific radiological dose in urban environments, accounting for complexity of the environment; 2) discovery of biosignatures of radiation exposure, as a function of time and dose for rapid assessment of human health impacts in a reliable manner; and 3) validation of human organ models as a physiologically relevant substitute to animal studies. Our project can resolve some of the big challenges in this field. Bioengineered organs will create a first ever capability to study radiation biology directly in human tissue. The suites of biomarkers identified could transform early exposure identification, and countermeasure development. Integration of modeling with experimentation will result in a unique human radiological dose capability for assessments across unprecedented scales. Thus, this project can integrate scientific innovation to actionable response and has the potential to initiate new research efforts in hazard response, training exercises for radiological disasters, and assessments for medical and decontamination communities.

Publications

Journal Articles

Akh, L. A., K. Scott, K. E. Coombs, A. Arefin, M. O. Ishak, H. J. Sandin, J. Huang, P. Nath, S. Iyer, R. S. Iyer and J. F. Harris. Development and Characterization of a Negative Pressure Fluidic Method for Lung-on-a-Chip Applications. Submitted to *Acta Biomaterialia*. (LA-UR-22-28557)

*Akh, L. A., M. O. Ishak, J. F. Harris, T. G. Glaros, Z. J. Sasiene, P. M. Mach, L. M. Lilley and E. M. McBride. -Omics potential of in vitro skin models for radiation exposure. 2022. *Cellular and Molecular Life Sciences*. **79** (7): 390. (LA-UR-22-22894 DOI: 10.1007/s00018-022-04394-z)

Brambilla, S., M. A. Nelson, P. T. Conry, N. Duboc and M. J. Brown. Dirty bomb source term characterization and downwind dispersion: review of experimental evidence. Submitted to *Journal of Environmental Radioactivity*. (LA-UR-21-31129)

Brambilla, S., M. A. Nelson and M. J. Brown. Dirty bomb source term characterization and downwind dispersion: review of experimental evidence. Submitted to *Journal of Environmental Radioactivity*. (LA-UR-23-21480)

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Klumpp, J. A., L. Bertelli, K. Eckerman, M. A. Nelson, L. R. Wedell, M. L. Deshler, S. Brambilla and M. J. Brown. Introducing DEPDOSE, a Tool to Calculate Inhalation Dose Coefficients to Members of the Public for Radioactive Aerosols. Submitted to *Health Physics*. (LA-UR-23-20254)

Livshits, M. Y., L. R. Stromberg, S. C. Moore, K. E. Aldrich, G. L. Wagner, S. A. Kozimor, H. Mukundan and L. M. Lilley. Growth Inhibition Effects of 227Th Alpha Emitter Metallated Siderophore Complexes on Pseudomonas aeruginosa. Submitted to *Journal of the American Chemical Society*. (LA-UR-22-33071)

Presentation Slides

Akhadov, L. E. Summary of Research Experience. . (LA-UR-21-30606)

Brambilla, S. and M. J. Brown. Relevance of Laboratory Data for Estimating Particle Resuspension from Outdoor Surfaces. Presented at *24th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling*, Fairfax, Virginia, United States, 2020-12-08 - 2020-12-10. (LA-UR-20-30022)

Coombs, K. E. Microphysiological Systems and Mechanobiology. . (LA-UR-21-23309)

Davis-Anderson, K. L. and K. Ganguly. Utilizing Microphysiological Systems to Decipher Biosignatures Following Radiation Exposure. Presented at *BioNuclear Working Group*, Lorton, Virginia, United States, 2023-02-28 - 2023-02-28. (LA-UR-23-21949)

Harris, J. F. Microphysiological Human Models for Biodosimetry. Presented at *JOWOG 43*, Lorton, Virginia, United States, 2022-09-19 - 2022-09-23. (LA-CP-22-20690)

Hetrick, L. D. Practical Overview of Monte Carlo N-Particle (MCNP) for a Health Physicist. . (LA-UR-22-25591)

Hetrick, L. D. Incorporating the ICRP 145 Mesh-Type Reference Computation Phantoms (MRCPs) into Urban Environments for Dose Calculations. Presented at *Weapons Effects Meeting*, Washington DC, District Of Columbia, United States, 2022-09-20 - 2022-09-23. (LA-UR-22-29285)

Ishak, M. O., K. A. Yu, B. H. Jun and J. F. Harris. Human Exposure of Radiation using Organ Systems Skin Model. . (LA-UR-22-31741)

Posters

Ishak, M. O., L. A. Akh, J. F. Harris, T. G. Glaros, Z. J. Sasiene, P. M. Mach, L. M. Lilley and E. M. McBride. In-vitro 3D Skin Model with Applications in Biodosimetry & Toxicology. Presented at *2022 Chemical and Biological Defense Science &Technology (CBD S&T) Conference*, San Francisco, California, United States, 2022-12-06 - 2022-10-09. (LA-UR-22-31548)

Jun, B. H., J. E. Torrez, M. O. Ishak, D. J. Ross, K. L. Davis-Anderson and J. F. Harris. Fabrication of a 3D-Printed Bone Marrow Bioreactor. Presented at *TERMIS-AM 2023 Annual Conference*, Boston, Massachusetts, United States, 2023-04-11 - 2023-04-14. (LA-UR-23-23436)

Moore, S. C., L. Lilley, G. L. Wagner, M. Y. Livshits, M. E. Moore, J. F. Harris and H. Mukundan. Chemical or Radiological Toxicity: Effects of Uranium Oxides on Human Lung Cells. Presented at *Society of Toxicology*, Nashiville, Tennessee, United States, 2023-03-19 - 2023-03-19. (LA-UR-23-22731)

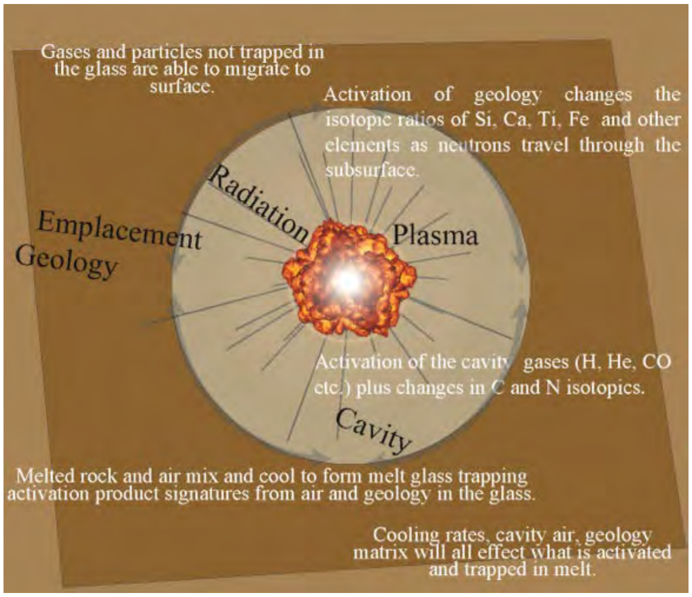
Moore, S. C., L. M. Lilley, G. L. Wagner, M. Y. Livshits, M. E. Moore, J. F. Harris and H. Mukundan. Chemical or Radiological Toxicity: Effects of Uranium Oxides on Human Lung Cells. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-02. (LA-UR-22-27640)

Moore, S. C., L. M. Lilley, H. Mukundan and J. F. Harris. Chemical or Radiological Toxicity: Effects of Uranium Oxides on Human Lung Cells. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, San Diego, California, United States, 2022-03-20 - 2022-03-20. (LA-UR-22-22533)

*Peer-reviewed

Basic Science of Underground Nuclear Explosions: Emplacement Condition Signature Discovery

Thomas Rahn
20210215DR



The project is using chemical analyses of underground nuclear explosive debris to determine the manner and sophistication in which a given test was carried out. The Figure displays an underground nuclear explosion with the multiple interactions of the radiation with the cavity air, emplacement geology and infrastructure that are being explored via analyses of resulting glass and minerals as well as trapped gases.

Project Description

The research proposed in this project will support national security and stockpile stewardship by increasing our understanding of the behavior of material surrounding an Underground Nuclear Explosion (UNE). Although many parts of a UNE have been studied, there are key gaps that warrant more research, and one of these will be explored as part of this project. Through both measurement of gaseous inclusions and actinide isotopes in debris plus simulations of up to thousands of isotopes generated during the event producing the debris, a comparative assessment of the results will indicate what areas we still need to study more thoroughly.

Publications

Reports

Gonzalez, E., J. C. Armstrong and J. R. Tutt. MCNP6.3 Unstructured Mesh Verification: GodivR and CANDU Models. Unpublished report. (LA-UR-22-33091)

Rahn, T. A., H. B. D. Miller and D. L. Eldridge. A CRUSHING AND GAS SEPARATION VACUUM LINE SYSTEM FOR THE PURIFICATION AND STUDY OF GASES IN ROCK SAMPLES. Unpublished report. (LA-UR-21-31695)

Presentation Slides

Boggs, M. A., A. A. Reinhard, J. D. Inglis, W. P. Brug, C. Margiotta and G. Lee. 135/137 Cesium Measurements in Various Forms of Trinitite by Thermal Ionization Mass Spectroscopy. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kailua-Kona, Hawaii, United States, 2022-04-03 - 2022-04-08. (LA-UR-22-22840)

Boggs, M. A., A. A. Reinhard, J. D. Inglis, W. P. Brug and G. Lee. 135/137 Cesium Measurements in Nuclear Debris: Applications to Nuclear Forensics. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, Indianapolis, Indiana, United States, 2023-03-26 - 2023-03-29. (LA-UR-23-22739)

Boukhalfa, H., A. Migdissov and C. E. Campe. Partitioning of Actinides and Metals Between the Vapor Phase and the Melt. . (LA-UR-21-31900)

Eldridge, D. L., H. B. D. Miller, T. A. Rahn, C. E. Campe, A. Migdissov and H. Boukhalfa. Gas Liberation, Detection, & Quantification from Geological, Experimental, & Nuclear Weapons Test Materials. . (LA-UR-23-20396)

Gonzalez, E. Unstructured Mesh: MCNP6.3 Verification. Presented at *KEEPIN summer 2022*, Los Alamos, New Mexico, United States, 2022-08-10 - 2022-08-10. (LA-UR-22-28229)

Gonzalez, E. MCNP6.3 Unstructured Mesh Verification: GodivR and CANDU Models. Presented at *summer student presentation on projects related to MCNP*, los alamos, New Mexico, United States, 2022-08-16 - 2022-08-16. (LA-UR-22-28575)

Reinhard, A. A., J. D. Inglis, A. H. S. Kara, S. J. Goldstein, D. M. Lopez, S. P. Lamont and R. E. Steiner. Utility of ATONA amplifiers for isotopic analyses by thermal ionization mass spectrometry. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kona, Hawaii, United States, 2022-04-03 - 2022-04-09. (LA-UR-22-22749)

Tutt, J. R. and T. C. McClanahan. Activation Calculations using MCNP Unstructured Mesh Geometries. Presented at *2021 MCNP\xc2\xae User Symposium (Virtual)*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26603)

Posters

Armstrong, J. C., J. R. Tutt and T. C. McClanahan. MCNP Unstructured Mesh Applications and Activation Calculations. Presented at *2021Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25742)

Armstrong, J. C., J. R. Tutt and T. C. McClanahan. MCNP Unstructured Mesh Applications and Activation Calculations. Presented at *2021Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25742)

Armstrong, J. C., J. R. Tutt and T. C. McClanahan. MCNP Unstructured Mesh Applications and Activation Calculations. Presented at *2021Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25742)

**Peer-reviewed*

Synthetic Opioid Detection: Stopping the Fentanyl Crisis at our Borders

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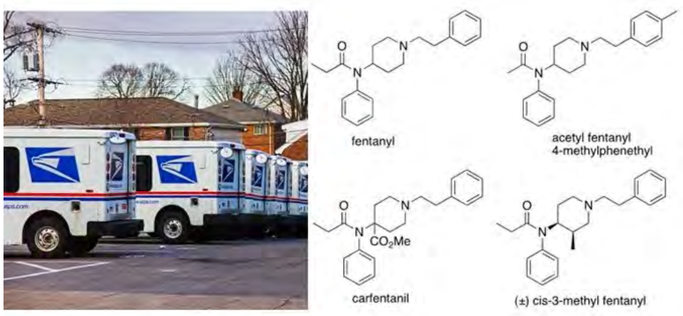
20220086DR



Deaths from drug overdose are at an all time record level. In order to stem the influx of one class of drugs, synthetic opioids, new instruments are needed to better probe the content of packages for illicit materials. Nuclear Quadrupole Resonance is one stand-off method that will be developed by this team. The challenge to be overcome is the multitude of fentanyl derivatives and the entire signature space that needs to be measured to help stop fentanyl from being shipped by postal services.

Project Description

To address the fentanyl health crisis and break the supply chain to our country, new approaches for screening packages and items at customs portals are necessary. A new technology needs to avoid pitfalls, positively identify all synthetic opioids, protect law enforcement from the dangerous contents, and provide a confidence level for the measurement. Nuclear Quadrupole Resonance (NQR) is an analytical technique that meets all of these requirements. This program will build the first standoff NQR detector of fentanyl with the approach combining our world-class team experienced in state-of-the-art instruments for detecting explosives and chemical warfare agents with cutting edge machine learning and artificial intelligence methods. These new capabilities could be transitioned to help the United States Postal Service (USPS) meet the requirements of the Synthetics Trafficking and Overdose Prevention (STOP) Act.

Publications

Journal Articles

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Klein, N. E., M. Malone, H. E. Mason, A. J. Day and S. Williamson. Denoising neural networks for magnetic resonance spectroscopy. Presented at *IEEE International Conference on Acoustics, Speech, and Signal Processing*. (Rhodes Island, Greece, 2023-06-04 - 2023-06-04). (LA-UR-22-30980)

Presentation Slides

Day, A. J. Complex-Valued Signal Denoising and Bayesian Optimization for Detection of Synthetic Opioids. . (LA-UR-22-31711)

Day, A. J., N. E. Klein, M. Malone, H. E. Mason and S. Williamson. Detecting synthetic opioids with NQR spectroscopy and complex-valued signal denoising. Presented at *LANL Student Symposium (virtual)*, Online, New Mexico, United States, 2022-08-01 - 2022-08-01. (LA-UR-22-27755)

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Malone, M., M. A. Espy, M. T. Janicke, N. E. Klein and R. F. Williams. CHALLENGES IN OBTAINING NQR PARAMETERS FROM FENTANYL CITRATE USING FAST FIELD CYCLING RELAXOMETRY. Presented at *12th Conference on Fast Field Cycling NMR Relaxometry*, cambridge, United Kingdom, 2022-07-13 - 2022-07-15. (LA-UR-22-26611)

Posters

Altenhof, A. R., D. C. Kaseman, H. E. Mason, M. A. Alvarez, M. Malone and R. F. Williams. On the Effects of Quadrupolar Relaxation in Earth's Field NMR Spectra. Presented at *Experimental NMR Conference (ENC)*, Pacific Grove, California, United States, 2023-04-16 - 2023-04-20. (LA-UR-23-23111)

Altenhof, A. R., S. M. Greer, S. G. Newman and M. Malone. Towards the Design and Implementation of a DNP-NQR Spectrometer. Presented at *Southeastern Magnetic Resonance Conference (SEMRC)*, Tallahassee, Florida, United States, 2022-11-04 - 2022-11-06. (LA-UR-22-31784)

Day, A. J., N. E. Klein, H. E. Mason, M. Malone and S. Williamson. Detecting Synthetic Opioids with Nuclear Quadrupole Resonance Spectroscopy and Denoising Neural Networks. Presented at *Annual Conference on Neural Information Processing Systems (NIPS)*, New Orleans, Louisiana, United States, 2022-11-27 - 2022-11-27. (LA-UR-22-32146)

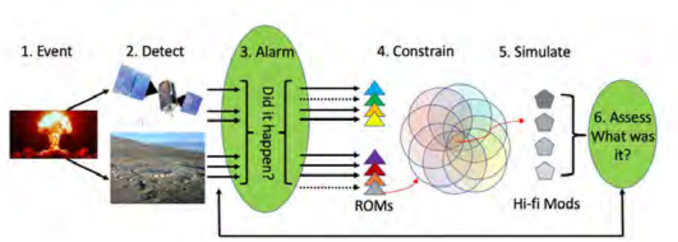
Day, A. J., N. E. Klein and S. Williamson. Detecting Synthetic Opioids with NQR Spectroscopy and Complex-Valued NNs. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-22384)

Malone, M. Nuclear Quadrupole Resonance for Synthetic Opioid Detection. Presented at *NMR**2*, Albuquerque, New Mexico, United States, 2021-10-30 - 2021-10-30. (LA-UR-21-30631)

**Peer-reviewed*

Integrated Nuclear Detonation Detection (iNDD)

Tracy Lavezzi Light
20220188DR



At present, each sensing phenomenology across space- and ground-based nuclear detonation detection programs treat each sensor trigger individually (incoming lines at step 3 of figure). This project will develop two further steps. First, a step to jointly assess all triggers in determining whether a likely nuclear event occurred. Such combined analysis will enable lower sensing thresholds while decreasing system-level triggers, for an overall increase in NDD system sensitivity. Second, a step to assess the event yield and location that also includes all available data, compared against high fidelity simulation, resulting in improved yield and location values that include uncertainty estimates.

Project Description

In the field of Nuclear Detonation Detection (NDD), the United States maintains significant remote sensing capability both on the ground and in space for global, continual treaty monitoring. Currently, the individual NDD program elements (for example, seismic and space-based detection) operate independently. This approach has three general shortcomings: (1) costly attempts to perfect individual sensors, (2) increased potential for false alarms, and (3) possible misleading interpretation due to single-sensor analysis. This project will drastically improve NDD capabilities by pioneering a multi-source, data fusion methods to harness the power of integration across the nation's multi-domain sensing infrastructure. Previous work (using only data collected by ground-based assets) has demonstrated the potential: joint consideration of multiple data streams (for example, combining seismic with infrasound) improves the reliability of event identification as nuclear or non-nuclear, while also limiting false alarms, improving full-system sensitivity, and improving assessment of event yield. In order to extend that work to consider ground-based and space-based data together, linking the entire NDD infrastructure, extensions and improvements to existing statistical methods are needed. This work will fill that gap and prototype a nuclear event monitoring system that maximizes the capability of the existing infrastructure.

Publications

Reports

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Presentation Slides

Blom, P. S. Defining a Mach cone source for infrasonic ray tracing analysis. . (LA-UR-22-30804)

Blom, P. S. Modeling regional propagation of infrasonic Mach cone energy from a supersonic source. Presented at *Acoustical Society of America (ASA) - Fall Meeting*, Nasvhille, Tennessee, United States, 2022-12-05 - 2022-12-09. (LA-UR-22-32448)

Carmichael, J. D. A Waveform Detection Tutorial: A (Very) Short Course. . (LA-UR-23-23408)

Carmichael, J. D., T. E. Lavezzi Light, R. A. Alfaro-Diaz, M. A. R. Kaltenborn, C. A. Kruschwitz and B. J. Williams. Data Fusion to Support Integrated Nuclear Detonation Detection (iNDD). . (LA-UR-22-29547)

Carmichael, J. D. and T. E. Lavezzi Light. Erratum to: Data Fusion to Support Integrated Nuclear Detonation Detection (iNDD, LA-UR-22-29547). . (LA-UR-22-32191)

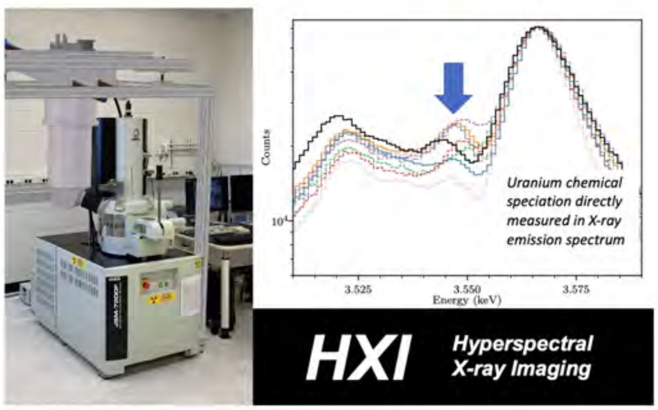
Posters

Delbridge, B. G., M. L. Begnaud, J. A. Kintner, R. T. Modrak, W. S. Phillips and J. D. Carmichael. Seismic yield estimation of the January 2022 Hunga-Tonga Eruption. Presented at *Seismological Society of America Annual Meeting*, Bellevue, Washington, United States, 2022-04-19 - 2022-04-23. (LA-UR-22-23551)

**Peer-reviewed*

Hyperspectral Xray Imaging (HXI): Nanochemical Analysis of Actinide and Explosive Materials

Mark Croce
20190002DR



Researchers at Los Alamos National Laboratory are developing a new capability for nanoscale chemical speciation mapping of small uranium and plutonium-containing samples: Hyperspectral X-ray Imaging (HXI). The chemical form of uranium or plutonium compounds is of particular importance to infer material history and origin for nuclear safeguards, environmental monitoring, and treaty verification. Subtle features in X-ray emission spectra (indicated by arrow) result from chemical effects such as oxidation state. By combining ultra-high-resolution microcalorimeter X-ray spectroscopy with the scanning electron microscope, HXI will bring capabilities to analytical laboratories that are only available at huge synchrotron facilities now.

Project Description

Small particles containing uranium compounds can come from almost anywhere in the nuclear fuel cycle or on the road to making a nuclear bomb. Characterization of their detailed chemical form is needed to understand potential material origins, history, and environmental fate. The International Atomic Energy Agency (IAEA) and the United States Air Force Technical Applications Center (AFTAC) have stated that chemical speciation, especially uranium oxidation state, is very important for small particles. Outside of the brightest light sources, mammoth synchrotron laboratories, there is no x-ray chemical analysis method that provides a comprehensive determination of actinide (uranium, plutonium) chemical form and the spatial resolution needed to study microscopic samples with nanoscale heterogeneity. We will develop the first comprehensive chemical analysis capability in a regular laboratory for such particles by combining ultra-high-resolution microcalorimeter x-ray detectors with a scanning electron microscope, and interpreting the data with advanced theoretical methods. There are few institutions in a position to fully implement this technology. Only Los Alamos is in a position to develop this technology for laboratory-based materials analysis, and only Los Alamos has a nuclear materials mandate. This project will create a new analytical capability to support national security priorities.

Technical Outcomes

The project successfully achieved its key objective of creating a new analytical capability for nanoscale uranium chemical speciation and highly sensitive elemental analysis of small actinide-containing particles in a scanning electron microscope. The team combined advances in low-temperature detector instrumentation, chemical science, and theory and data interpretation to enable measurement of subtle features in the X-ray emission spectrum resulting from uranium speciation and associate them with predicted electron transitions.

Publications

Journal Articles

Bright, E. L., L. Xu, M. L. Harding, R. Springell, A. C. Walters, M. Sundermann, M. Garcia-Fernandez, S. Agrestini, E. R. Batista, P. Yang, R. Caciuffo, G. van der Laan and H. G. Lander. Resonant inelastic x-ray scattering of U3O8 and UN. Submitted to *Physical Review B*. (LA-UR-22-25892)

Carpenter, M. H., B. Stein, K. E. Koehler, C. J. Fontes, C. M. Smith, G. L. Wagner, Z. K. Baker, M. L. Handley, M. W. Rabin, P. Yang, E. R. Batista, D. G. McNeel, K. A. Schreiber, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. S. Swetz, D. R. Schmidt, D. T. Becker, J. A. B. Mates, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels and M. P. Croce. Hyperspectral X-ray Imaging: Progress Towards Chemical Analysis in the SEM. Submitted to *IEEE Transactions on Applied Superconductivity*. (LA-UR-20-28609)

Carpenter, M. H., M. P. Croce, Z. K. Baker, E. R. Batista, M. P. Caffrey, C. J. Fontes, K. E. Koehler, S. E. Kossmann, K. G. McIntosh, M. W. Rabin, B. W. Renck, G. L. Wagner, M. P. Wilkerson, P. Yang, M. D. Yoho, J. N. Ullom, D. A. Bennett, G. C. O'Neil, C. D. Reintsema, D. R. Schmidt, G. C. Hilton, D. S. Swetz, D. T. Becker, J. D. Gard, J. Imrek, J. A. B. Mates, K. M. Morgan, D. Yan, A. L. Wessels, R. H. Cantor, J. A. Hall and D. T. Carver. Hyperspectral X-ray Imaging with TES Detectors for Nanoscale Chemical Speciation Mapping. 2020. *Journal of Low Temperature Physics*. **200** (5-6): 437-444. (LA-UR-19-27148 DOI: 10.1007/s10909-020-02456-9)

Li, J., L. Xu, M. Garcia-Fernandez, A. Nag, H. C. Robarts, A. C. Walters, X. Liu, J. Zhou, K. Wohlfeld, J. van den Brink, H. Ding and K. Zhou. Unraveling the Orbital Physics in a Canonical Orbital System KCuF3. 2021. *Physical Review Letters*. **126** (10): 106401. (LA-UR-20-27035 DOI: 10.1103/PhysRevLett.126.106401)

Yadav, R., L. Xu, M. Pizzochero, J. van den Brink, M. I. Katsnelson and O. V. Yazyev. Electronic excitations and spin interactions in chromium trihalides from embedded many-body wavefunctions. Submitted to *submitted to npj Computational Materials and posted on https://arxiv.org/abs/2208.02195*. (LA-UR-22-28234)

Conference Papers

Teti, E. S., S. Salazar Escobedo and M. H. Carpenter. Naive data mining and machine learning for high resolution, sparse x-ray spectra. Presented at *SPIE Applications of Machine Learning*. (San Diego, California, United States, 2022-08-23 - 2022-08-25). (LA-UR-22-27723)

Reports

Xu, L., S. L. Adelman, A. S. Ditter, J. M. Kasper, J. Su, G. T. Seidler, S. K. Cary, S. A. Kozimor, P. Yang and E. R. Batista. Revealing bonding nature of uranium complexes: from X-ray absorption to resonant inelastic scattering. Unpublished report. (LA-UR-22-31661)

Presentation Slides

Batista, E. R., P. Yang and L. Xu. Prediction of XES spectra for molecular systems. Presented at *LDRD Review*, Los Alamos, New Hampshire, United States, 2020-08-11 - 2020-08-11. (LA-UR-20-26148)

Carpenter, M. H., M. P. Croce, B. Stein, D. G. McNeel, K. A. Schreiber, J. Ullom, D. Bennett, J. A. B. Mates, J. Gard, J. Imrek, D. Becker, A. Wessels and K. Morgan. Ultra-High-Resolution Cryogenic X-ray Spectrometer for Advanced Electron Microscope Actinide Material Mapping (Hyperspectral X-ray Imaging). Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kailua-Kona, Hawaii, United States, 2022-04-03 - 2022-04-03. (LA-UR-22-23097)

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Croce, M. P. New Analytical Capabilities with Microcalorimeters. . (LA-UR-19-27141)

Croce, M. P. Microcalorimeter Technology for Enhanced Safeguards Capabilities. Presented at *INMM-ESARDA-INMMJ Workshop*, Tokyo, Japan, 2019-10-07 - 2019-10-07. (LA-UR-19-29984)

Croce, M. P. IAEA Sample Results and Microcalorimeter Capabilities. . (LA-UR-19-30668)

Croce, M. P. Non-Destructive Evaluation Capabilities with Calorimetry and Microcalorimetry. Presented at *2019 Pit CEPPC*, Los Alamos, New Mexico, United States, 2019-06-19 - 2019-06-19. (LA-UR-19-30824)

Croce, M. P. LANL LTD Projects. . (LA-UR-19-31710)

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Croce, M. P., M. H. Carpenter, K. E. Koehler, D. G. McNeel, K. A. Schreiber, C. M. Smith and S. L. Weidenbenner. Low-Temperature Detectors for High-Precision Measurements. . (LA-UR-21-24545)

Koehler, K. E. Microcalorimeters: A Bright, Bold Future. Presented at *SeeLANL*, Los Alamos, New Mexico, United States, 2020-01-13 - 2020-01-13. (LA-UR-20-20224)

Koehler, K. E. Microcalorimeters: A Bright, Bold Future. . (LA-UR-21-23649)

Koehler, K. E. and C. J. Fontes. Spectral Calculations of X-ray Emission for Microcalorimeter Measurements: Theoretical basis for small mystery peaks in experimental x-ray measurements. Presented at *MetroMMC Stakeholder Meeting*, Saclay, France, 2019-10-24 - 2019-10-24. (LA-UR-19-30853)

McNeel, D. G. Microcalorimeters: Versatile High-resolution Radiation Detectors. . (LA-UR-22-27221)

Schreiber, K. A. Phase Transitions near Absolute Zero: From the Quantum Hall Effect to Gamma Ray Detectors in the Dilution Refrigerator. Presented at *Purdue University Department of Physics Colloquium - Raman Prize for Graduate Students*, Online, Indiana, United States, 2021-04-22 - 2021-04-22. (LA-UR-21-23619)

Teti, E. S., S. Salazar Escobedo and M. H. Carpenter. Na \xc3\xafve Data Mining and Machine Learning for High Resolution, Sparse X-ray Spectra. Presented at *SPIE Applications of Machine Learning*, San Diego, California, United States, 2022-08-22 - 2022-08-25. (LA-UR-22-28850)

Xu, L. Ab initio modeling of the X-ray absorption and resonant inelastic scattering of actinides and d-metal systems. Presented at *Virtual seminar in Lawrence Berkeley National Lab*, Los Alamos, New Mexico, United States, 2022-09-01 - 2022-09-01. (LA-UR-22-29057)

Xu, L. Ab initio modeling of the X-ray absorption and resonant inelastic scattering of d-metal and actinide systems. Presented at *Virtual seminar at National Institute of Standards and Technology*, Los Alamos, New Mexico, United States, 2023-02-07 - 2023-02-07. (LA-UR-23-21091)

Xu, L., J. M. Kasper, M. P. Croce, S. A. Kozimor, E. R. Batista and P. Yang. Revealing bonding nature of uranium complexes: From X-ray absorption to resonant inelastic scattering. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Fall*, Chicago, Illinois, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28711)

Posters

Carpenter, M. H., K. E. Koehler, C. J. Fontes, D. G. McNeel, K. A. Schreiber, C. M. Smith, G. L. Wagner, B. Stein, E. G. Bowes, P. Yang, E. R. Batista, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. S. Swetz, D. R. Schmidt, D. T. Becker, J. A. B. Mates, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels, J. Webber and M. P. Croce. Hyperspectral X-ray Imaging: Next-Generation TES Microcalorimeters on the SEM. Presented at *Low-Temperature Detectors 19*, Virtual, New Mexico, United States, 2021-07-19 - 2021-07-30. (LA-UR-21-26481)

Carpenter, M. H., K. G. McIntosh, J. N. Ullom, D. A. Bennett, D. S. Swetz, C. D. Reintsema, J. D. Gard, D. T. Becker, J. A. B. Mates, K. M. Morgan, J. Imrek, A. L. Wessels and M. P. Croce. Development of a Wide-Range X-ray Emission Spectroscopy Measurement System with Transition Edge Sensors and Microwave Multiplexed Readout. Presented at *Low Temperature Detectors 18*, Milan, Italy, 2019-07-22 - 2019-07-26. (LA-UR-19-26750)

Carpenter, M. H., K. G. McIntosh, K. E. Koehler, C. J. Fontes, C. M. Smith, G. L. Wagner, Z. K. Baker, M. L. Handley, M. W. Rabin, M. P. Wilkerson, M. D. Yoho, P. Yang, E. R. Batista, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. S. Swetz, D. R. Schmidt, D. T. Becker, J. A. B. Mates, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels and M. P. Croce. Hyperspectral X-ray Imaging: First Results and Future Development. Presented at *Applied Superconductivity Conference (ASC) 2020*, Virtual, New Mexico, United States, 2020-10-25 - 2020-11-06. (LA-UR-20-28160)

Croce, M. P., Z. K. Baker, E. R. Batista, M. P. Caffrey, M. H. Carpenter, C. J. Fontes, K. E. Koehler, S. E. Kossmann, S. A. Kozimor, K. G. McIntosh, M. W. Rabin, B. W. Renck, G. L. Wagner, P. Yang, M. D. Yoho, M. P. Wilkerson, D. T. Becker, D. A. Bennett, J. D. Gard, J. Imrek, J. A. B. Mates, K. M. Morgan, G. C. O'Neil, C. D. Reintsema, D. R. Schmidt, D. S. Swetz, A. L. Wessels, J. N. Ullom, R. H. Cantor, J. A. Hall and D. T. Carver. Hyperspectral X-ray Imaging. Presented at *18th International Workshop on Low Temperature Detectors*, Milan, Italy, 2019-07-22 - 2019-07-22. (LA-UR-19-26600)

Koehler, K. E., C. J. Fontes, E. R. Batista, M. H. Carpenter, S. A. Kozimor, K. G. McIntosh, C. M. Smith, G. L. Wagner, P. Yang and M. P. Croce. Dirac-Fock-Slater Calculations for Low Intensity X-ray Features. Presented at *International Workshop on Theory Frontiers in Actinide Sciences*, Santa Fe, New Mexico, United States, 2020-02-02 - 2020-02-05. (LA-UR-20-20828)

McNeel, D. G., M. H. Carpenter, B. Stein, K. E. Koehler, C. J. Fontes, C. M. Smith, G. L. Wagner, M. L. Handley, M. W. Rabin, P. Yang, E. R. Batista, K. A. Schreiber, E. G. Bowes, M. P. Croce, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. Swetz, D. R. Schmidt, J. A. B. Mates, D. T. Becker, J. C. Weber, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels and Z. K. Baker. Progress toward absolute calibration of x-ray TESs. Presented at *19th International Workshop on Low Temperature Detectors*, Online, New Mexico, United States, 2021-07-19 - 2021-07-29. (LA-UR-21-26488)

McNeel, D. G., M. H. Carpenter, K. A. Schreiber, M. P. Croce, J. N. Ullom, D. A. Bennett, J. A. B. Mates, D. T. Becker, J. D. Gard, K. M. Morgan, J. Imrek and A. L. Wessels. Actinide chemical speciation from ultra-high-resolution cryogenic x-ray emissions spectroscopy. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kailua-Kona, Hawaii, United States, 2022-04-03 - 2022-04-08. (LA-UR-22-23040)

Teti, E. S. and M. H. Carpenter. Data-Driven Automatic Calibration (DDAC) Routine for High-Energy-Resolution X-ray Emission Spectroscopy. Presented at *Conference on*

Data Analysis (CoDA), Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-21974)

Xu, L., S. L. Adelman, A. S. Ditter, J. M. Kasper, S. K. Cary, S. A. Kozimor, P. Yang and E. R. Batista. Revealing bonding nature of uranium complexes: From X-ray absorption to resonant inelastic scattering. Presented at *Theory Frontiers in Actinide Science: Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21853)

Other

Carpenter, M. H. and M. P. Croce. HXI X1 Data as of November 2019. Dataset. (LA-UR-19-31890)

**Peer-reviewed*

Science of Signatures

Directed Research
Final Report

Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter

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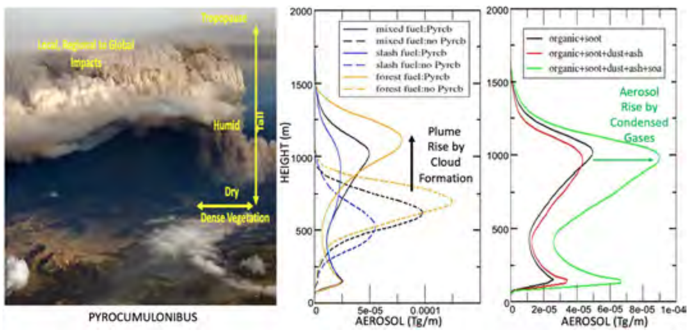
20200035DR



This project investigates post-blast urban fire smoke impact (e.g. fallout and nuclear winter) to minimize any collateral damage from a low-yield exchange. The image includes the vertical evolution of the smoke from a Pyrocumolonimbus (PyroCb system (left); simulations of the vertical profile of 2017 British Columbia PyroCb smoke illustrating the additional lofting by the mixed fuels and the latent heat released by the cloud formation (middle); and simulations showing that organic gas condensation in the cool updraft make secondary aerosols that can more than double the aerosol mass injected in the upper troposphere and lower stratosphere.

Project Description

The growing threat of a limited nuclear exchange demands 21st century science-tools to assess collateral damage from radioactive fallout that is lethal to humans and potential nuclear winter that could threaten habitability. Nuclear winter is the long-term solar shading, cooling, and drying simulated by global models that prescribe a high-altitude injection of soot form urban fires ignited by the exchange, and is very uncertain. It results from a large fraction of the dark smoke being self-lofted into the stratosphere by solar heating where it can persist for years. In contrast, if the smoke is injected at lower altitudes it rains out rapidly with no nuclear winter. However, in this case the smoke that is mixed with radioactive debris is transported to the surface over long range posing a health hazard. Our goal is to realistically treat the mixing, injection, fate, and transport of mixed smoke-dust produced by low yield exchange for robust assessments. Laboratory measurements of the chemical, optical and microphysical properties of dust-smoke particles using state-of-the-art instruments will be incorporated into our multi-phenomenology fireball, neutron activation, fire, and global atmospheric models. Finally, validation simulations for available observations on 2017 Pacific Northwest megafires and Hiroshima black-rain will be performed.

Technical Outcomes

The project performed the first ever experimentally based multi-phenomenology end-to-end simulations of Pyrocumulonumbus stratospheric mass injections that treat fire dynamics, particle sources, their lofting and long-range transport by interactions with moisture, ice, convection, synoptic weather and sunlight to reproduce the observed features. Results elucidated complex wildfire smoke processes and demonstrated that forecasting them with close to real time data assimilation is necessary to predict any potential for nuclear winter that is missing in past assessment.

Publications

Journal Articles

*Aiken, A. C., R. C. Huber, A. M. Schmalzer, M. Boggs, J. E. Lee, K. J. Gorkowski, D. W. Podlesak and M. K. Dubey. High temperature and pressure regime soot: Physical, optical and chemical signatures from high explosive detonations. 2022. *Aerosol Science and Technology*. **56** (10): 931-946. (LA-UR-22-23547 DOI: 10.1080/02786826.2022.2105686)

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*Chylek, P., C. Folland, J. D. Klett and M. K. Dubey. CMIP5 Climate Models Overestimate Cooling by Volcanic Aerosols. 2020. *Geophysical Research Letters*. **47** (3): e2020GL087047. (LA-UR-19-32146 DOI: 10.1029/2020GL087047)

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Dubey, M. K., K. J. Gorkowski and S. Guerin. Looking Within the Medio Fire Smoke Plume at Los Alamos National Laboratory. . (LA-UR-20-26772)

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Aiken, A. C., M. K. Dubey, J. E. Lee, R. C. Huber and T. L. Williamson. Detonation Soot Chemistry using High Time-Resolution Aerosol Mass Spectrometry. Presented at *Carbon in Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-10-28 - 2019-10-28. (LA-UR-19-31002)

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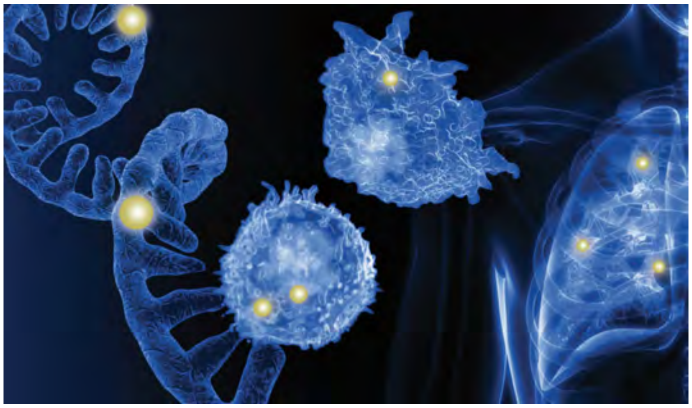
**Peer-reviewed*

Capturing the Origin and Evolution of Persistence Using Real-Time, In Vivo, Single Cell Transcriptomics

Murray Wolinsky
20200222DR



This image was taken from the on-line Los Alamos Workshop on Visualizing Living Systems, conducted by our project on February 25, 2021. This effort pushes the frontiers of visualization of important biochemical processes (specifically the transcription of information from deoxyribonucleic acid (DNA) to messenger ribonucleic acid (mRNA)) enabling much deeper insight into how cells operate and achieve their ends. The ultimate goal of the project is to facilitate real-time "conversations" between experimenters and their cellular objects of study.

Project Description

Antimicrobial and anticancer therapies frequently fail due to tiny numbers of cells which persist despite treatment. Current analysis (transcriptomic) methods are blind to the existence and behavior of these crucial actors ("persisters") unless infeasible numbers of cells are employed. Improving therapies requires developing new methods. Our effort will identify and study the persisters that determine the fate of populations using novel technology developed for that purpose. Existing methods of transcriptomics are inadequate. But a radically new approach has only recently become possible: the ability to monitor the internal state of individual cells and to do this for many cells in real time. We will mature this latent technology, drawing on critical Los Alamos innovations. Our project is organized to perform foundational studies using our transformational new approach. We will observe the temporal dynamics of gene expression in single cells in vivo. Our method is called RIVOT (Real-time In VivO Transcriptomics). We will identify each gene expression event of interest by generating bar-coded signals as it occurs. We will watch expression of multiple (~10) targeted genes simultaneously. Our effort will not only provide unprecedented insight into persistence, it will revolutionize the study of gene expression in doing so.

Technical Outcomes

Novel mechanisms of regulating bacterial persistence, potentially leading to better therapeutics were identified. A new system for studying persistence in human cancer cells was developed and used to discover a mechanism of cancer stress response. New means of labelling deoxyribonucleic acid (DNA) in vivo were designed with commercial potential. Progress was made toward developing new semi-synthetic organisms which incorporate unnatural base pairs (UBPs) in their life cycle, including techniques for synthesizing and exploiting the UBPs.

Publications

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Reports

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Presentation Slides

Banerjee, S. and R. K. Jha. Transporter Modeling and Design For Designer Cargo. Presented at *Visualizing Living Systems*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21867)

Bolding, M. R. Persistence in Cancer. Presented at *Workshop on Visualizing Living Systems*, Virtual, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21823)

Bolding, M. R., D. P. Morales and N. Pace. A new nucleic acid labeling strategy using biarsenical dyes. . (LA-UR-22-31723)

Bolding, M. R., N. Pace and D. P. Morales. A new nucleic acid labeling strategy using biarsenical dyes. . (LA-UR-22-29902)

Corbin, J. R., R. Wu and J. G. Schmidt. Synthetic Chemistry to Support RIVOT. Presented at *Workshop on Visualizing Living Systems*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21866)

Hennelly, S. P. Engineering a Semi-synthetic Organism for Real-time detection of Gene expression.. Presented at *Visualizing Living Systems Workshop*, LOS ALAMOS, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21711)

Hennelly, S. P. Engineering a Semi-synthetic Organism for Real-time detection of Gene expression.. Presented at *Worksop on Visualizing Living Systems*, LOS ALAMOS, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22011)

Kumar, A., S. P. Hennelly and N. A. Pace. Integration and Maintenance of unnatural base pairs (UBPS) Inside the Living Cell. Presented at *Workshop on Visualizing Living Systems draft agenda*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22580)

Morales, D. P., S. N. Micheva-Viteva, M. A. Wolinsky and J. H. Werner. Measuring gene expression involved in bacterial persistence at the single cell level. Presented at *Visualizing Living Systems Workshop*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21719)

Pace, N. A., P. M. Goodwin, S. P. Hennelly and R. Wu. FRET Gate for Real-Time In-Vivo Transcription. Presented at *Visualizing Living Systems Workshop*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22692)

Werner, J. H. Methods to Visualize 3D Dynamics. Presented at *Northern Arizona University Seminar*, Virtual, New Mexico, United States, 2020-10-22 - 2020-10-22. (LA-UR-20-28259)

Wolinsky, M. A. welcome and Introduction to the LANL Workshop on Visualizing Living Systems. Presented at *LANL Workshop on Visualizing Living Systems*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22713)

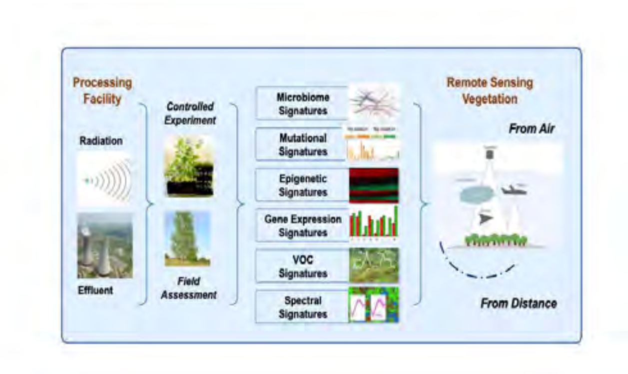
Posters

Micheva-Viteva, S. N. and E. Hong-Geller. In Pursuit of Effective Host-Directed Therapies Against Human Pathogens. Presented at *CBD&T Conference*, Cincinati, Ohio, United States, 2019-11-18 - 2019-11-22. (LA-UR-19-31135)

**Peer-reviewed*

BioSignatures for Nuclear Nonproliferation: Plants as a Bio-Sentinel System

Helen Cui
20220669DR



Nuclear facility activities and effluents generate physical and chemical signals and induce changes in the surrounding biological systems, especially in plants because of their immobility. The stress responses in affected vegetation can take place at different levels from molecular to systematic scale, which can potentially be measured and quantified, and detected by a variety of sensing methods. Gene expression and epigenetic profiles can be a key link associating with multi-phenomenological changes in plants, taking a priority for this LDRD research. The methods and findings pave a path to comprehensive design and development for an integrated plant bio-sentinel signature discovery.

Project Description

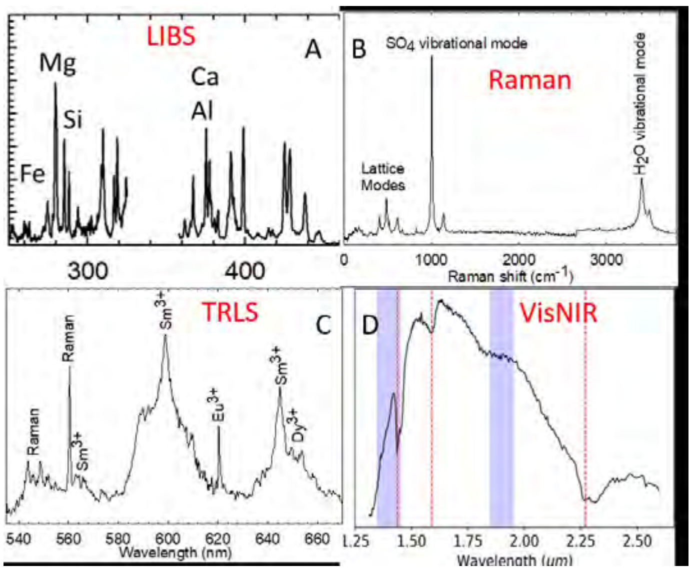
Detecting nuclear proliferation activities at different stages is critical to United States policy makers and national security stakeholders. However, current research and development (R&D) activities and investments in nonproliferation detection and monitoring have been focused on physics- and chemistry-based methods, less on non-traditional approaches. We believe that proliferation monitoring, detection, and verification can benefit from transformative sensing methods. Vegetation is a uniquely well-suited candidate as a bio-sensor, for its immobility, and intrinsic abilities to respond and survive environmental changes. A systematic study will enable characterization of nuclear facility effluent related vegetation signals, and development of quantitative sensitive signatures and field monitoring capability. Our ultimate goal is to develop capabilities to discover bio-signatures from natural vegetation that can be correlated with nuclear facility activities and effluents, and detected by remote sensing. In this innovative project, we will launch a pilot study to investigate vegetation molecular regulatory response and genetic structural modifications under selected test conditions. We will develop an initial analytic workflow, by integrating modern sequencing technologies, bioinformatics analysis, and machine learning and artificial intelligence (AI) algorithms; and integrate remote sensing capacities for vegetation phenomenological signals. The research methods and findings can be extended to chem/bio nonproliferation, and contribute to fundamental scientific disciplines.

Technical Outcomes

The research team successfully conducted multi-module experiments and analyses examining responses of two broadly existing sorghum species to different gamma-irradiation exposure conditions. The study identified specific gene expression patterns in Sorghum halepense and Sorghum bicolor that are dose- and time-dependent. The team developed a robust and streamlined method to assess complex stress signaling using portable spectrometry, and examined the feasibility and challenges of using volatile organic compound measurement.

The Advanced Mission Relevant Science Enabled by a Build-to-Print Mini-Intensified Charge Coupled Device (ICCD) Detector

Samuel Clegg
20220670DR



Quantitative molecular and elemental analysis from a single instrument enables one to distinguish anthropogenic and natural materials. Remote molecular or chemical analysis can be readily accomplished but acquiring both from a single, portable instrument in a remote configuration is rare. This project will demonstrate that a single instrument can remotely collect elemental (Laser-Induced Breakdown Spectroscopy (LIBS, A), Time-Resolved Luminescence Spectroscopy (TRLS, C)), and molecular (Raman (B), Visible and Near Infrared (VisNIR, D)) spectra of global security related samples.

Project Description

Quantitative chemical speciation and elemental analysis from a single instrument enables one to distinguish anthropogenic and natural materials. A single, portable instrument that can remotely collect both molecular and elemental information is rare. This project will demonstrate that a single instrument can remotely characterize the elemental and molecular composition of several sample classes important to the global security mission. A miniature intensified charge coupled device (ICCD) detector enables this unique capability. This project will also mature this detector into a build-to-print device. The results of this project will also enable transformational advances in many Los Alamos National Laboratory and Department of Energy mission areas.

Technical Outcomes

This project completed both of the proposed tasks. First, we demonstrated the complementary diagnostic data that can be determined by an integrated elemental and molecular analysis. The capability to collect both of these signatures requires sensitive detectors. Second, we completed the design of a miniature intensified charge coupled device (ICCD) detector that enables the integrated detection of elemental and molecular signatures by Laser-Induced Breakdown Spectroscopy (LIBS) and Raman spectroscopy.

Publications

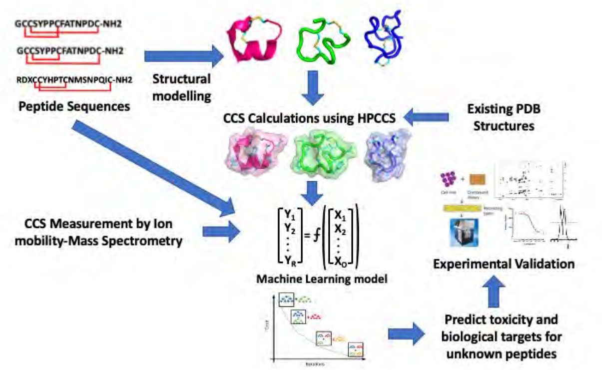
Reports

Zhang, Y. First-principles simulation of molecular qubits for quantum information (w22_mofqis): annual report. Unpublished report. (LA-UR-23-23230)

**Peer-reviewed*

A New Approach to Predict Toxicity of Small Molecule Toxins

Hau Nguyen
20210172ER



Despite the recognized and important roles of small molecule- and peptide-based toxins in novel therapeutic treatments, our ability to identify, characterize, and determine the toxicities of small molecule- and peptide-based toxins is difficult, costly, and time-consuming. By developing a platform of integrated modeling/experimental tools and a machine learning-based predictive model, the capability to predict the toxicity and biological targets of a molecule based on experimentally or computationally determined Collisional Cross Section (CCS) values that represent the size, shape, and sequence of a toxin provides a paradigm shift from traditional cellular toxicology and animal studies leading to faster and more reliable therapeutic outcomes.

Project Description

Biochemical agents, and toxin molecules in particular, pose one of the greatest threats to our national security, as shown by multiple attempts in recent decades to poison government officials in the United States and Great Britain. Devising effective means to identify and screen for toxins from environmental samples is thus a crucial component of modern national security measures. Unlike radiological threat agents, toxins appear inert in the environment, and only display their functionality once ingested or absorbed by an organism, making them a dangerously insidious form of potential terrorism that requires advanced identification measures. By developing analytical methods that can rapidly identify toxins by their molecular structure, and thus avoid the need for testing functionality on living systems, we will be able to screen environments for toxin molecules in high-throughput and identify the expected toxicity of an environment. This research also has the potential to inform the development of novel therapeutics with similar molecular structures and functionality. Thus our methods will benefit national security as well as development of new therapeutics for medical treatment.

Publications

Journal Articles

B. Nguyen, H. T., G. S. Waldo and T. C. Terwilliger. Engineering an Efficient and Bright Split Corynactis Californica Green Fluorescent Protein. Submitted to *Scientific Reports*. (LA-UR-21-25224)

B. Nguyen, H. T., L. Huynh, G. Gupta, J. Vel\xc3\xa1squez, R. Rabara and S. Basu. Rational design of antimicrobial peptides targeting Gram-negative bacteria. Submitted to *Computational Biology and Chemistry*. (LA-UR-21-20035)

Presentation Slides

Carver, D. T., D. W. Brown, T. R. Jacobs, A. I. Smith, J. Park and P. Kenesei. High Energy X-Ray Characterization of Microstructure at Macroscopic Depths in Pu Alloys. Presented at *Pu Futures 2022*, Avignon, France, 2022-09-26 - 2022-09-29. (LA-UR-22-29679)

Miner, J. C. Combined experimental / computational characterization of small biotoxin structures. . (LA-UR-21-22118)

Miner, J. C. Characterizing RNA molecules through high-performance computing. . (LA-UR-21-26081)

B. Nguyen, H. T., R. F. Williams, P. M. D. Truong, L. K. Monroe, S. H. Adikari and J. Miner. A New Platform to Predict Toxicity and Biological Targets of Small Molecule Toxins. Presented at *DTRA 2022 CBD S&T Conference*, San Francisco, California, United States, 2022-12-06 - 2022-12-09. (LA-UR-22-31402)

B. Nguyen, H. T. and L. K. Monroe. T22_Toxin Viewgraph. . (LA-UR-23-23337)

**Peer-reviewed*

Science of Signatures

Exploratory Research
Continuing Project

Long-lived Fauna as Tracers of Anthropogenic Radionuclides

Cyler Conrad
20210220ER

Tortoises and turtles growth sequential layers on their scute (keratin) tissue across their bony shell. These layers grow like tree rings, often in annual layers. The desert tortoise (Gopherus agassizii) shown in this photograph, from the Nevada National Security Site, has several of these sequential rings present on their scute. The LDRD team is sampling individual layers of tortoise/turtle scute tissue – among other animal tissues with similar growth histories – to identify the presence of anthropogenic radionuclides from nuclear testing and production activities worldwide. [Image credit: Derek Hall, Nevada National Security Site]

Project Description

Historic, legacy radionuclide records from the era of above ground nuclear testing are difficult to capture and analyze. Using long-lived animal skeletons curated in museum collections, specifically tortoises and turtles, we plan to analyze radionuclides which are deposited on a yearly basis within tortoise shell to understand anthropogenic radionuclide incorporation into this animal and tissue type from the Trinity Test Site, Nevada Test Site, in Kazakhstan and in the Galapagos. Our challenge is to find new ways to track radionuclides in the environment, especially to further the goals of nuclear forensics and non-proliferation programs within the Department of Energy and other associated federal agencies. If we are successful in identifying and analyzing annual records of radionuclides from tortoise/turtle shell tissue, we expect that this technique will be valuable in aiding radionuclide identification from nuclear testing or processing facilities/activities, and clandestine passive collecting approaches.

Publications

Journal Articles

Conrad, C. N., J. D. Inglis, A. M. Wende, M. E. Sanborn, N. Mukundan, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, E. A. Middlebrook, S. M. Gaukler, J. J. Whicker, J. L. Gerard, W. T. Aguilera, J. P. Gibbs, B. Wolf, K. de Brum, M. Hagemann, J. Seminoff, T. Brys, R. Brown and K. Derieg. Nuclear Contamination in Sequentially Grown Turtle Scute. Submitted to *Nature*. (LA-UR-22-24577)

Conrad, C. N., J. D. Inglis, J. J. Whicker and J. L. Gerard. Allometric-kinetic model predictions of radionuclide dynamics across turtle species. Submitted to *Environmental Pollution*. (LA-UR-22-29197)

Presentation Slides

Conrad, C. N., A. M. Wende, J. D. Inglis, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, S. M. Gaukler, J. J. Whicker, W. T. Aguilera, J. P. Gibbs and B. Wolf. Long-lived Fauna as Tracers of Anthropogenic Radionuclides. . (LA-UR-20-29525)

Conrad, C. N., A. M. Wende, J. D. Inglis, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, S. M. Gaukler, J. J. Whicker, W. Tapia Aguilera, J. Gibbs and B. Wolf. Tracing the legacy of anthropogenic radionuclides from 20th Century nuclear testing in desert tortoises (Gopherus agassizi) at the Nevada Test Site. Presented at *Desert Tortoise Council*, Tuscon, Arizona, United States, 2021-02-16 - 2021-02-16. (LA-UR-21-21186)

Conrad, C. N., J. D. Inglis, N. Mukundan, A. M. Wende, M. E. Sanborn, Z. Macsik, A. A. Price, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, E. A. Middlebrook, S. M. Gaukler, J. J. Whicker, J. L. Gerard, W. T. Aguilera, J. Gibbs and B. Wolf. LDRD ER Appraisal: Long lived Fauna as Tracers of Anthropogenic Radionuclides (20210220ER). . (LA-UR-23-20964)

Conrad, C. N., J. D. Inglis, N. Mukundan, A. M. Wende, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, E. A. Middlebrook, S. M. Gaukler, J. J. Whicker, W. T. Aguilera, J. P. Gibbs and B. Wolf. Tortoises and Turtles as Passive Collectors of Anthropogenic Radionuclides from Nuclear Testing and Production Activities. Presented at *Turtle Survival Alliance*, Charleston, South Carolina, United States, 2021-08-13 - 2021-08-13. (LA-UR-21-27883)

Inglis, J. D. Analysis of Turtle and Tortoise Scutes can Provide a Time-Constrained Record of Radionuclide Releases into the Environment. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, kailua-Kona, Hawaii, United States, 2022-04-04 - 2022-04-04. (LA-UR-22-22272)

Inglis, J. D. Instruments, Forensics, Turtles & Hot Sauce: The Role of an Isotope Geochemist at LANL. . (LA-UR-22-30693)

Wurth, K. N., T. J. Tenner, B. E. Naes and C. N. Conrad. SIMS Uranium Isotope Analysis of NIST Standard Glasses to Determine Detection Limits. Presented at *Microscopy and Microanalysis*, Portland, Oregon, United States, 2022-08-01 - 2022-07-28. (LA-UR-22-26096)

Posters

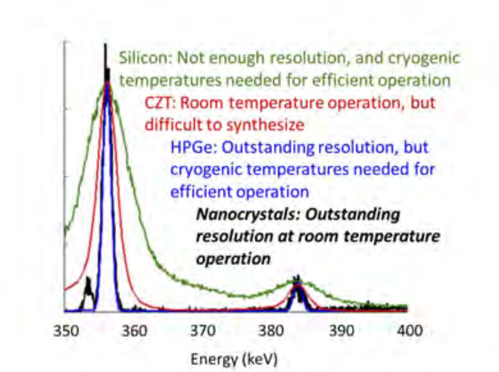
Inglis, J. D., A. A. Reinhard, M. A. Boggs, A. H. S. Kara and J. Louis Jean. Highly sensitive isotope ratio measurements in support of nuclear non-proliferation, safeguards and nuclear forensic programs.. Presented at *Science of Signatures 2022 Review*, Los Alamos, New Mexico, United States, 2022-04-11 - 2022-04-14. (LA-UR-22-23084)

Mukundan, N., J. D. Inglis and C. N. Conrad. Nuclear Contamination in Sequentially Grown Turtle Scute. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-02 - 2022-08-02. (LA-UR-22-27620)

**Peer-reviewed*

Identification of Gamma Radiation Enabled by Semi-Conductive Nanocrystalline Materials

Amanda Graff
20210253ER



Quickly and accurately identifying a radioactive source is challenging. Current state-of-the-art radiation detectors, such as silicon, cadmium zinc telluride (CZT), and HPGe (high-purity germanium) suffer serious shortcomings that hamper their use in real-world applications. In collaboration with researchers at the University of Michigan, researchers at Los Alamos National Lab are investigating the performance and applicability of nanocrystalline-based radiation detectors. Preliminary reports in the literature suggest that nanocrystalline-based radiation detectors operate at room temperature with high resolution, making such detectors more attractive for real-world applications than currently available options. [Image credit: LANL and University of Michigan]

Project Description

The current limitations of nuclear material detection and identification can be viewed largely as a function of the sensing materials used in radiation detectors. Not only have commonly used materials have been technologically stagnant for decades, they either are expensive to produce on a large scale or require cryogenic temperatures for efficient operations. Our research will lay the groundwork for the development of radiation detectors that address current shortcomings. Our goal is to produce radiation detectors not only capable of quickly detecting and identifying radioactive material without cumbersome cooling equipment, but also at a lower cost than state-of-the-art commercial detectors. Successful execution of this project will have a direct impact on every activity that is dependent on fast and accurate identification of not only special nuclear material (SNM). Such activities include nonproliferation, counter-proliferation, and emergency response efforts.

Publications

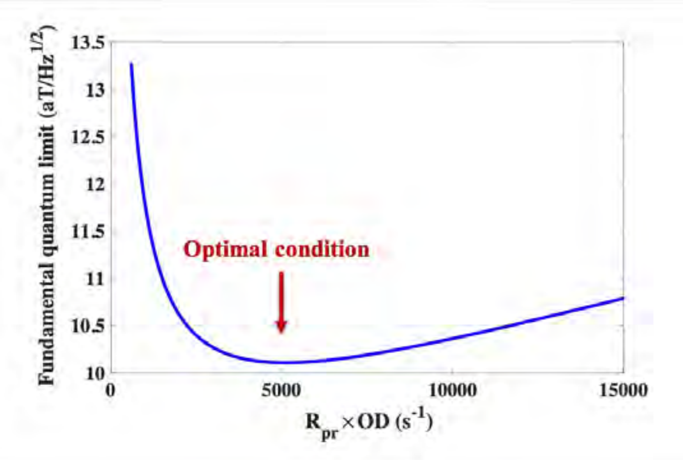
Posters

Grunau, S. E. Quantum Dots for Enhancement of Scintillating Radiation Detection. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Online, New Mexico, United States, 2022-08-02 - 2022-08-03. (LA-UR-22-27558)

**Peer-reviewed*

Most Sensitive Optical Quantum Sensor

Young Jin Kim
20210254ER



The key challenge in various ultra-sensitive magnetic field measurements, such as fundamental physics searches and biomedical research, is to overcome the sensitivity limitation of the existing sensor technology. This project will demonstrate an innovative approach to develop by far the most sensitive optical quantum sensor reaching 10 aT sensitivity beyond the capability of current technology in high-frequency magnetic field detection.

Project Description

This project will result in a new high-frequency optical quantum sensor (OQS) with sensitivity reaching the fundamental quantum limit, beyond the capability of current technology in magnetic field detection. The new sensor technology would address the sensor sensitivity limitation problem in many existing high-precision magnetic field measurements by improving the sensitivity of the best available commercial magnetic sensors by more than two orders of magnitude. The advanced OQS will contribute to the grand scientific challenge of discovering new physics beyond the Standard Model of particle physics, supporting the Laboratory's fundamental science mission and Nuclear and Particle Futures science pillar. This project will also provide opportunities to develop the talent pipeline and technology supporting the Laboratory's national security mission.

Publications

Journal Articles

Savukov, I. M. and Y. J. Kim. Broadband Ultra-sensitive Adiabatic Magnetometer. Submitted to *IEEE Sensors*. (LA-UR-21-24891)

Presentation Slides

Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)

Kim, Y. J., I. M. Savukov, P. Chu, L. D. Duffy and S. G. Newman. Fundamental Physics Searches using Atomic Magnetometers. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-30 - 2022-06-03. (LA-UR-22-24823)

Kim, Y. J., I. M. Savukov, P. Chu, S. G. Newman and L. D. Duffy. Optically Pumped Magnetometers and Their Applications in Fundamental Physics Searches. Presented at *Aps April Meeting*, New York, New York, United States, 2022-04-09 - 2022-04-12. (LA-UR-22-23153)

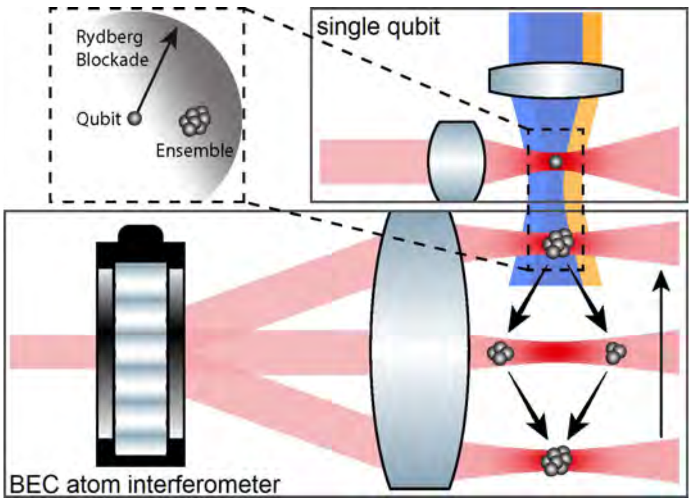
Posters

Kim, Y. J. and I. M. Savukov. Applications of Optically Pumped Magnetometers in Fundamental Physics and Biophysics. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22087)

**Peer-reviewed*

Atom Interferometry Without Coherence

Katarzyna Krzyzanowska
20210301ER



Atom interferometers using ultracold atom matter waves can be exquisite sensors of gravity, acceleration, and rotation. The latter is important for navigation in GPS-denied environments. The sensitivity of a standard atom interferometer is limited by classical noise. Our project will exploit quantum physics (e.g. entanglement) to increase the measuring sensitivity by orders of magnitude. The figure shows how the atom interferometer (bottom) interacts through a quantum computing protocol known as DQC1 with a single excited atom trapped in a focused laser beam (top left and top right). The enhanced evolution of that single qubit is the sensor output.

Project Description

The National Quantum Initiative recognizes the importance to the Nation of quantum information technologies such as quantum sensing. We have developed a rotation sensor that will eventually enable accurate navigation when a Global Positioning System (GPS) is denied or unavailable. That is a pressing challenge facing both the Defense and Intelligence communities. The sensor can also be configured to measure gravitational fields, which has applications to nonproliferation. This project will use a protocol originally developed for quantum computing to enhance the performance of our sensor beyond the usual boundaries imposed by noise, which will have high impact on the areas above.

Publications

Journal Articles

Zurek, W. H. Quantum Theory of the Classical: Einselection, Envariance, and Quantum Darwinism. Submitted to *Entropy*. (LA-UR-21-31822)

Presentation Slides

Calder, C. M. Automation and Machine Learning for Robust and Self-Tuning Magneto-Optical Traps. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27580)

Calder, C. M. Automation and Machine Learning for Robust and Self-Tuning Magneto-Optical Traps. Presented at *EERE AMO Internships Summer Presentation*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-27748)

Girolami, D., A. Touil, B. Yan, S. Deffner and W. H. Zurek. Quantitative limits to quantum correlations in many-body systems: a signature of classical objectivity. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21970)

Krzyzanowska, K. A. Atom gyroscopes - exploiting quantumness of cold atoms for sensing. Presented at *IOP Lecture hosted by The Open University*, Milton Keynes, United Kingdom, 2022-04-13 - 2022-04-13. (LA-UR-22-23398)

Krzyzanowska, K. A. Atom interferometry 1.0 and 2.0 for inertial sensing. Presented at *Quantum Sensing Workshop 2023 at Lawrence Berkeley National Laboratory*, Berkley, California, United States, 2023-02-14 - 2023-02-16. (LA-UR-23-21562)

Martin, M. J. Ultracold atom-based quantum technologies at LANL. Presented at *RPI/LANL Nucleation Workshop on Quantum Materials and Devices*, Los Alamos, New Mexico, United States, 2022-04-29 - 2022-04-29. (LA-UR-22-23851)

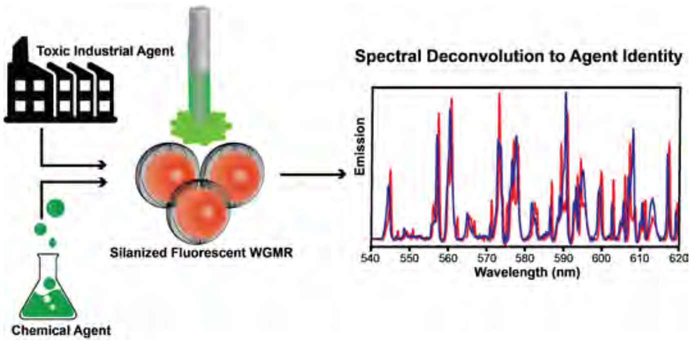
Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

Zurek, W. H. Information Scrambling, Loschmidt Echo,and Decoherence. . (LA-UR-21-29934)

**Peer-reviewed*

Whispering-Gallery-Resonator Beads for Rapid and Sensitive Chemical Threat Detection

Benjamin Stein
20210367ER



Optical detection of chemical threat agents (such as sarin) or toxic industrial agents (such as isocyanate) via interactions with functionalized (silica shelled) whispering gallery mode resonator (WGMR) microspheres results in emission intensities with sub-nm wavelengths. Real signals of fluorescent microspheres in different media have sub-nanometer widths (right) to enable single or multiplex analysis after deconvolution and signal processing. These unique, interpretable spectra incorporated into a spectral library can yield rapid, selective, in-field agent identity

Project Description

Chemical threat and toxic industrial agents pose a threat to national security. Fortunately, outside of World War I there have been limited modern examples of chemical agent (clandestine or otherwise) use. There have, however, been several modern examples of devastating toxic industrial agent accidents including the Seveso disaster in 1976 and the Bhopal India release in 1989. The global expansion of commodity and pharmaceutical industries greatly expands access to these agents and presents a need for technological advancement in chemical threat detection/identification. We will address CBRNE (Chemical, Biological, Radiological, Nuclear, and high yield Explosives) threat reduction efforts by improving detection strategies for chemical signatures. This research focuses on a new fieldable detection method with unparalleled gas detection multiplexing. Whispering gallery mode resonator microspheres (functionalized for chemical threat agent detection) offer a potent solution to challenges currently present in the detection of chemical threats in highly complex mixtures. Further, we are building a robust signal processing and spectral library infrastructure that will enable this technology to be deployable. Facilitating rapid, sensitive, and selective multiplexed detection methods for such agents serves the dual role of providing a proof-of-concept while addressing the national and international need.

Publications

Journal Articles

*Paulus, B. C., J. K. Banh, K. D. Rector, B. W. Stein and L. M. Lilley. Whispering gallery mode resonators in continuous flow: spectral assignments and sensing with monodisperse microspheres. 2022. *Analytical Methods*. **14** (17): 1690-1697. (LA-UR-21-30848 DOI: 10.1039/D2AY00181K)

Presentation Slides

Lilley, L. M. Journey to the National Laboratory. . (LA-UR-20-30040)

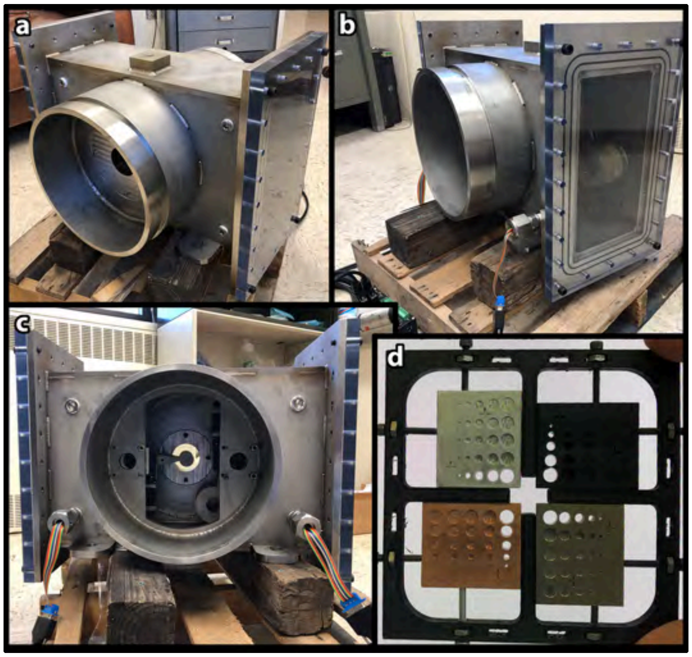
Posters

Paulus, B. C., J. K. Banh, K. D. Lenz, K. D. Rector, B. Stein and L. M. Lilley. Continuous Flow Measurements of Whispering Gallery Mode Spectra for Characterization of Microsphere Resonators and their Local Environment. Presented at *ACS Spring 2022 Bonding Through Chemistry*, San Diego, California, United States, 2022-03-20 - 2022-03-24. (LA-UR-22-22227)

**Peer-reviewed*

Dark Field Proton Radiography

William Meijer
20210419ER



The project will implement a robust and fully automated device to adjust the parameters for dark field proton radiography. The device will allow for an improvement of workflow, and a better optimization of future experiments. Above, images A-C shows the completed collimator apparatus with two coordinated, rotating stages that set the collimator to one of eight possible settings. This will enable instantaneous collimator swap capability at a time savings of four hours per swap, unlocking new capabilities and efficiencies in pRad operations. The images show the assembly as prepared for static testing. Image D shows the multi-material multi density test pattern, constructed of tungsten, steel, copper, and aluminum, with a variety of resolution (both spatial and density) features, that will allow for the full calibration of the system using a single object in the field of view.

Project Description

Proton radiography (pRAD) typically operates in a very high density regime, aquiring 21 imaging frames on a 200-nanseconds (ns) timescale, while other imaging modalities are either well suited for visualizing thinner objects, or do not have the temporal capabilities of pRad. This development seeks to broaden the applicability of pRad by visualizing thinner processes on a fast timescale, and to improve the workflow of the pRad facility by streamlining what is now a time consuming process: adjusting collimator (transmission) settings. The goal of this project is to evaluate a very subtle, but fast system, such as the mixing of high-Atwood number gases under pressure loading. It is expected that we will optimize this system to be better able to visualize such low-contrast processes, and that we will streamline the workflow at pRad to allow for quicker shot-to-shot turnaround through the automated, blast-proof collimator assembly that we will provide.

Publications

Journal Articles

Broder, B. A., E. F. Aulwes, M. A. Espy, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. S. Freeman. A TOPAS model for lens-based proton radiography. Submitted to *Medical Physics*. (LA-UR-21-28343)

Broder, B. A., E. F. Aulwes, M. A. Espy, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. S. Freeman. A TOPAS model for lens-based proton radiography. Submitted to *Physics in Medicine and Biology*. (LA-UR-22-20784)

Reports

Meijer, W. Z. Dark Field Proton Radiography Los Alamos LDRD Report. Unpublished report. (LA-UR-23-22486)

Presentation Slides

Freeman, M. S. Charged Particle Radiography as an HED Diagnostic. Presented at *41stInternational Workshop on High Energy-Density Physics with Intense Laser Beams*, Virtual, New Mexico, United States, 2021-02-01 - 2021-02-01. (LA-UR-21-21038)

Posters

Broder, B. A. and M. S. Freeman. ASSESSMENT OF CLINICAL TO HIGH ENERGY PROTON RADIOGRAPHY VIABILITY USING TOPAS. Presented at *American Association of Physicists in Medicine Annual Meeting*, Virtual, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-27482)

Meijer, W. Z., J. C. Allison, E. F. Aulwes, D. C. Cardon, M. S. Freeman, F. E. Merrill, R. B. Sidebottom and M. A. Espy. Increasing the Proton Radiography Sensitivity to Material Shock Front Detection. Presented at *22nd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK22)*, anaheim, California, United States, 2022-07-10 - 2022-07-10. (LA-UR-22-26171)

**Peer-reviewed*

Listening for Rock Coatings on Mars: Using Acoustic Signals from Laser-Induced Breakdown Spectroscopy

Nina Lanza
20210424ER

LDRD researchers use a large thermal-vacuum environmental chamber to learn more about how sound propagates on Mars. The SuperCam instrument on board the NASA Perseverance rover includes a rock-ablating laser and a microphone. Analyses by the laser create an acoustic signal ("zap") that the microphone records. The acoustic signal can identify rock coatings, an important target in the search for past life on Mars. This experimental chamber back on Earth provides a large volume of Mars-like atmosphere in which similar acoustic experiments may be performed, allowing for a more accurate interpretation of acoustic data returned by SuperCam from Mars.

Project Description

Rock coatings are a key place in which to search for signs of life on Mars, which is a major goal of the National Aeronautics and Space Administration (NASA) Perseverance Mars rover. The Los Alamos led SuperCam instrument suite onboard Perseverance is highly suited for the study of rock coatings because it includes both a laser-induced breakdown spectroscopy (LIBS) instrument and a microphone to record the zapping sound of LIBS laser sparks. By examining both the chemical and acoustic signals obtained by LIBS, the presence and nature of a rock coating may be positively identified. The goal of this work is to identify rock coatings in a Mars-like environment using the acoustic signals (zapping sounds) from laser-induced breakdown spectroscopy analyses. The proposed work will position Los Alamos at the forefront of an emerging field of study by laying the foundation for a new type of analysis for natural rocks, as well as building fundamental knowledge about LIBS acoustics and sound propagation on Mars.

Publications

Conference Papers

Larmat, C., E. R. Dauson, A. L. Reyes-Newell, A. M. Ollila, J. A. Ten Cate, B. Chide, N. L. Lanza and R. C. Wiens. Using Laboratory LIBS Acoustics Experiments to Elucidate SuperCam Microphone Data on Mars.. Presented at *53rd Lunar and Planetary Science Conference*. (Woodlands, Texas, United States, 2022-03-07 - 2022-03-11). (LA-UR-22-20251)

Presentation Slides

Dauson, E. R. Acoustic signals from laser-induced breakdown spectroscopy: Listening for coatings on Martian rocks. . (LA-UR-20-30175)

Larmat, C., E. R. Dauson, A. M. Ollila, J. A. Ten Cate, B. Chide, A. L. Reyes-Newell, N. L. Lanza and R. Wiens. Using Laboratory LIBS Acoustics Experiments to Elucidate SuperCam Microphone Data on Mars.. Presented at *2022 SCiX*, Covington, Kentucky, United States, 2022-10-03 - 2022-10-07. (LA-UR-22-30265)

Rolland, L., C. Larmat, O. Karatekin, A. Spiga, E. Samson, B. Fernando, G. Sainton and P. Lognonn\xc3\xa9. Sonic Booms from Atmospheric Entries. Presented at *2021 AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31936)

Rolland, L., C. Larmat and O. Karatekin. Sonic Boom and Impact Acoustics on Mars and Earth. Presented at *22th InSight Science Team Meeting*, Online, New Mexico, United States, 2021-10-25 - 2021-10-29. (LA-UR-21-30644)

Rolland, L., O. Karatekin and C. Larmat. Sonic Booms from spacecraft entries, a Mars/Earth perspective. Presented at *InSight Science Team Meeting 21-2021*, online, New Mexico, United States, 2021-06-28 - 2021-07-01. (LA-UR-21-26087)

Posters

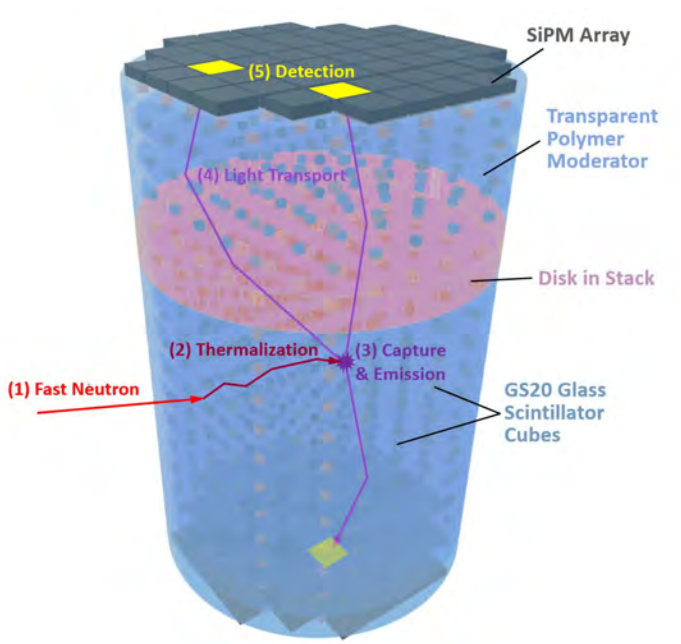
Larmat, C., E. R. Dauson, A. L. Reyes-Newell, A. M. Ollila, J. A. Ten Cate, B. Chide, N. L. Lanza and R. C. Wiens. USING LABORATORY LIBS ACOUSTICS EXPERIMENTS TO ELUCIDATE SUPERCAM MICROPHONE DATA ON MARS.. Presented at *53th Lunar and Planetary Science Conference*, Online, New Mexico, United States, 2022-03-07 - 2022-03-11. (LA-UR-22-21971)

Larmat, C., E. R. Dauson, A. M. Ollila, J. A. Ten Cate, B. Chide, V. J. Vigil, N. L. Lanza and R. C. Wiens. Non-linearity Observed in Laboratory LIBS Acoustic Experiments.. Presented at *2022 AGU Fall meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32507)

**Peer-reviewed*

High Dynamic Range Neutron Detector for Pulsed Applications

Markus Hehlen
20210431ER



Neutron detection in a solid-state composite: an incident fast neutron (1) is thermalized in the polymer moderator (2) and captured by lithium (Li)-6 in small glass cubes that emit scintillation light (3) which propagates through the transparent moderator (4) and is detected by silicon photomultiplier (SiPM) arrays on the surface. Reading out the SiPMs in both photon-counting and photo-current mode enables the detector to achieve a linear response over a large range of incident neutron fluxes. The project aims at demonstrating a 5000 times higher dynamic range than helium (He)-3 detectors for the same detection efficiency.

Project Description

A short pulse of neutrons arriving at a remote detector is a highly valuable signature of a nuclear event as it carries information about the intensity, dynamics, and energetics of the source. The remote measurement of a short neutron pulse is essential to the Space-based Nuclear Detonation Detection (SNDD) program supporting DOE's treaty verification mission. It is also a key capability for the Neutron Diagnosed Subcritical Experiment (NDSE) and Enhanced Capabilities for Subcritical Experiments (ECSE) programs in support of the Stockpile Stewardship mission. Traditional helium-3 (He-3) tubes suffer from a limited dynamic range. We aim to overcome this limitation by exploring and demonstrating a new type of neutron detector that is expected to have a ~5000× higher dynamic range than He-3 detectors for the same detection efficiency. The detector combines a composite scintillator with a high-dynamic range readout of silicon photomultipliers. We will explore and develop a high dynamic range calibration scheme, parallel readout of silicon photomultipliers, and an optically transparent composite scintillator. We expect these research themes to yield several publications and new patent applications. The successful completion of the proposed work will establish the multi-disciplinary knowledge base that will enable us to propose a subsequent application-specific detector development.

Publications

Journal Articles

Richards, C. G., B. W. Wiggins, M. Iliev, A. Favalli, T. D. Mclean, A. Gomez and M. P. Hehlen. Performance Assessment of a Compact Neutron Detector Module Based on Scintillating Composites. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-22-27235)

Wiggins, B. W., M. P. Hehlen, R. O. Nelson and C. G. Richards. Optical transport simulations in radiation damaged scintillating particle composite systems. Submitted to *Journal of Applied Physics*. (LA-UR-19-29565)

Presentation Slides

Richards, C. G., B. W. Wiggins, M. Iliev, A. Favalli, T. D. Mclean, A. Gomez and M. P. Hehlen. Performance Assessment of a Compact Neutron Detector Module Based on Scintillating Composites. Presented at *International Society for Optics and Photonics (SPIE) Optics and Photonics Conference*, San Diego, California, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28628)

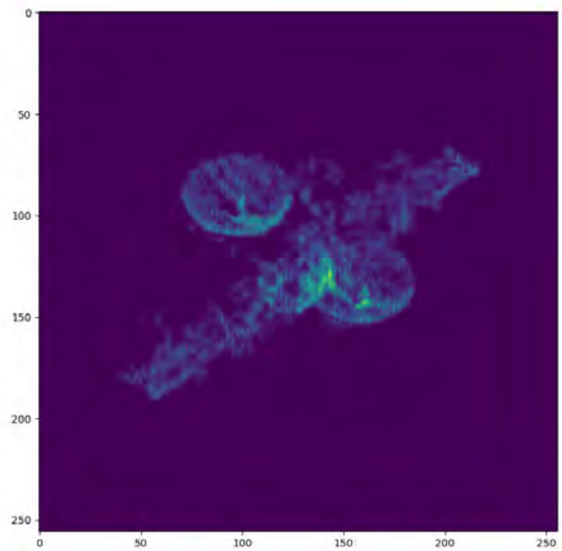
Wiggins, B. W., , C. G. Richards, M. Iliev, A. Favalli, N. K. Wehmann, T. D. Mclean and M. P. Hehlen. Fast Neutron Detection Using Scintillating Composites. Presented at *SCINT 2022*, Santa Fe, New Mexico, United States, 2022-09-19 - 2022-09-23. (LA-UR-22-29404)

Wiggins, B. W., C. G. Richards, M. Iliev and M. P. Hehlen. Compact-High Dynamic Range Composites for Space Applications. Presented at *TECH TALK*, Los Alamos, New Mexico, United States, 2021-08-09 - 2021-08-09. (LA-UR-21-30343)

**Peer-reviewed*

Using Laser Synthetic Aperture Radar to Image a Low Earth Orbit Satellite

Mitchell Hoffmann
20210435ER



Three-dimensional image of a satellite, based on simulated laser ranging data. Imaging satellites that are many hundreds, or thousands, of kilometers above the ground, is very challenging but also very important for maintaining and protecting important space assets. The project seeks to demonstrate a novel imaging concept that could potentially achieve cm-scale imaging resolution at extremely long range, far beyond the current state-of-the-art.

Project Description

We have developed a novel imaging concept that could potentially achieve centimeter-scale imaging resolution at extremely long range, far beyond current state-of-the-art. This concept uses a modified radar technique, but illuminating the target with a laser and measuring the round-trip time of laser photons instead of radar emissions. We have already tested the technique on the ground at ranges up to 10 kilometer (km), and demonstrated better spatial resolution than that of a conventional imaging radar. We propose to demonstrate this imaging technique on a space object for the first time by laser-illuminating a satellite in low earth orbit (at a range of 500-1000km) from the Air Force Research Laboratory's Starfire Optical Range (SOR) in Albuquerque, and detecting return photons on the ground (also at SOR), as the satellite angle changes during a pass overhead. The experiment will further develop the experimental technique and the required data analysis techniques. Future mission areas that could be enabled by this research include space treaty verification, planetary defense against earth colliding asteroids, and missile defense. This novel imaging approach has transformational impact, enabling new classes of long-range, high-resolution imaging missions for both national security and basic science.

Publications

Journal Articles

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. C. Thompson and D. Palmer. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Submitted to *Applied Optics*. (LA-UR-21-29582)

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. Palmer and D. C. Thompson. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Submitted to *Applied Optics*. (LA-UR-21-32462)

Presentation Slides

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. C. Thompson and D. Palmer. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Presented at *Imaging and Applied Optics Congress*, Vancouver, Canada, 2021-07-19 - 2021-07-23. (LA-UR-21-22050)

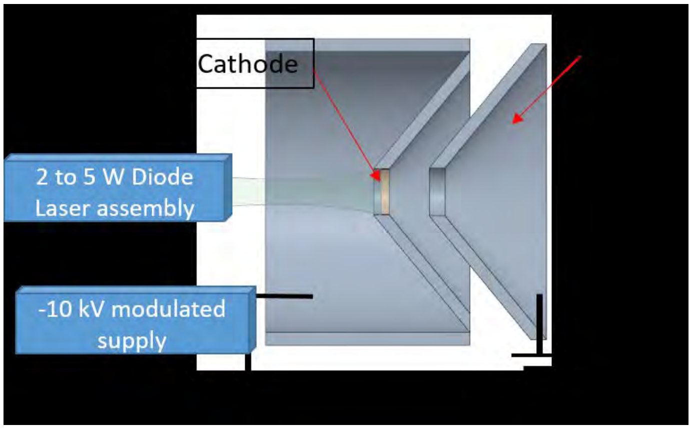
Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. C. Thompson and D. Palmer. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Presented at *OSA Imaging and Applied Optics Congress*, Vancouver, Canada, 2021-07-19 - 2021-07-23. (LA-UR-21-26408)

Thompson, D. C. and J. A. Cox. Los Alamos National Laboratory Intelligence and Space Research Division. . (LA-UR-22-22551)

**Peer-reviewed*

A Low Power Electron Injector for Space Applications

Darrel Beckman
20210443ER



The image above is a simple block diagram of the project team's injector design concept. The injector consists of a thermionic cathode for the electron source, a laser to heat the cathode and control electron emission current, and a high voltage power supply (HVPS) to provide potential for accelerating electrons into a beam line. By heating the cathode with a laser the team will decouple the heating element from the HVPS thereby simplifying the electronics design and reducing power requirements. The 10 kilovolt supply is designed for space flight applications using an innovative technique for designing and building transformers using embedded printed circuit board (PCB) windings.

Project Description

One threat that could cripple critical space infrastructure is high energy electrons from solar wind or high altitude nuclear explosions that become trapped in the Earth's radiation belts. These electrons can cause electrostatic buildup and discharge on satellites causing critical damage. Radiation belt remediation is an important area of research being conducted at Los Alamos National Lab. One promising approach to mitigate this threat is to generate electromagnetic waves using a modulated electron beam from an accelerator in orbit. The work of this project is critical technology development of an electron source that will be required to develop an orbital electron accelerator to meet future radiation belt remediation experiments and operational missions. The electron source design innovations in this work will reduce complexity, improve efficiency and mechanical robustness, and will be scalable to meet future mission needs.

Publications

Reports

Santana, G. N. and D. T. Beckman. LANL INTERNSHIP LEARNING OBJECTIVES. Unpublished report. (LA-UR-22-28328)

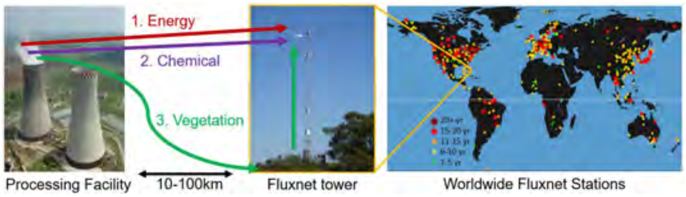
Posters

Andrews, H. L., A. M. Alexander, D. T. Beckman, A. S. Guider, M. A. Holloway, J. P. Moody, J. C. J. Moreno and G. N. Santana. Initial Results from a Laser-Heated Thermionic Cathode. Presented at *Advanced Accelerator Concepts Workshop (AAC)*, Hauppauge, New York, United States, 2022-11-07 - 2022-11-11. (LA-UR-22-31698)

**Peer-reviewed*

Ecosystem Functional Signatures for Remote Proliferation Detection

Ann Junghans
20220062ER



Conceptual use of Fluxnet data for monitoring nuclear processing facilities with three proposed signature pathways, and map of active Fluxnet station locations with operation duration indicated by color. While some geographic areas of interest have relatively few stations, the network is constantly growing by ~ 10s of stations per year for applications such as carbon trading.

Project Description

This research will lay the foundation to harness a readily available, near-real-time datastream from a global ecosystem monitoring network as a means for remote proliferation detection. Signature extraction will not require any sample preparation and may allow for remote, non-obvious detection of proliferation activities. Apart from growing the already existing network, obtaining and expanding this datastream will not require any instrument deployment or sample collection. This datastream will provide a supplementary source to help reduce uncertainties in interpretation of Comprehensive Nuclear-Test-Ban Treaty data, and may allow for detection of different nuclear activity sources, from power plants to underground complexes. The method could be of particular interest for use in developing countries and Africa, where many countries are only starting to utilize nuclear power for civilian use and rely on foreign entities (mainly Russia/China) in their nuclear reactor operations. In these regions, potential inaccuracy of declared nuclear material and nuclear-related activities adds a new level of complexity to nuclear treaty verification. While the Fluxnet network does not currently cover all locations of interest, coverage world-wide is increasing because of growing interests in global carbon emission trading and could easily be expanded through facilitation of, for example, citizen science projects.

Publications

Journal Articles

Nakad, M., S. A. Sevanto, J. C. Domec and G. Katul. Linking the water and carbon economies of plants in a drying and warming climate. Submitted to *Current Forestry Reports*. (LA-UR-23-21278)

Reports

Peterman, A. B. Accessing Information from Environmental Monitoring Stations to Monitor Nuclear Facility Status. Unpublished report. (LA-UR-22-24854)

Presentation Slides

Peterman, A. B. Accessing Information from Environmental Monitoring Stations to Monitor Nuclear Facility Status. . (LA-UR-22-24851)

Posters

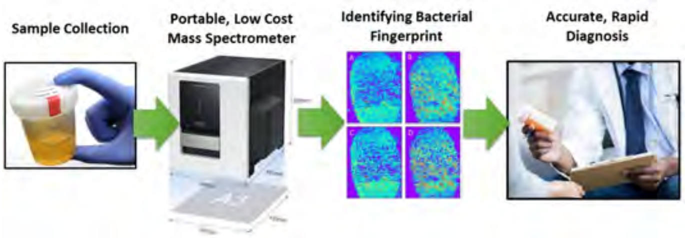
Kraklow, V. A., L. T. Dickman, S. A. Sevanto, E. M. Casleton and A. S. Junghans. Detecting nuclear effluent signatures at FluxNet ecological monitoring stations. Presented at *Conference on Data Analysis (CoDA)*, Sant Fe, New Mexico, United States, 2023-03-07 - 2023-02-09. (LA-UR-23-21919)

Nakad, M., L. T. Dickman, E. M. Casleton, S. A. Sevanto and A. S. Junghans. Ecosystem functional signatures for remote proliferation detection - identifying flux footprints. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, los alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27251)

**Peer-reviewed*

Multi-Dimensional Portable Mass Spectrometry for Biological Detection

Ethan McBride
20220088ER



A suspect sample containing a biological pathogen can be analyzed on a low cost portable mass spectrometer to generate a unique multidimensional mass fingerprint that allows for identification and, if clinical in nature, a rapid diagnosis which is essential to prescribe the correct medication.

Project Description

Over the last two decades, there has been an explosion of rapid detection and diagnostic assays which can be used in the field or at the bedside. Most of these technologies are antibody or genomic-based which can be fraught with false positives and negatives, require prior knowledge regarding the causative organism, and are easily compromised via genetic engineering or through naturally acquired mutations. Mass spectrometry (MS) technologies have been demonstrated to have best-in-class sensitivity and specificity for the detection and identification of pathogens in clinical settings utilizing an approach known as mass fingerprinting. These costly Food and Drug Administration approved instrument platforms are not designed to operate outside of a laboratory thus limiting widespread deployment. Portable, low-cost MS systems exist today for the detection and quantification of chemical warfare agents, but compromises for portability have limited their utility for biological detection. In this project, we will leverage and improve existing portable miniaturized instrument designs by implementing and validating a new data acquisition mode that enables us to acquire high fidelity data despite current technological limitations required for biological identification. These innovations will revolutionize our ability to detect biological threats a priori and result in a paradigm shift for point-of-care medicine.

Publications

Presentation Slides

Glaros, T. G. Mass Spectrometry Center for Integrated Omics. Presented at *Innovations in Mass Spectrometry*, Los Alamos, New Mexico, United States, 2022-08-10 - 2022-08-11. (LA-UR-22-28304)

McBride, E. M., Z. J. Sasiene, T. G. Glaros, W. S. Hlavacek, N. Velappan, E. S. LeBrun, J. Norris, R. Caprioli, N. H. Patterson, M. Dufresne and M. Farrow. Multidimensional Portable Mass Spectrometry for Biological Detection. Presented at *Workshop on Harsh-Environment Mass Spectrometry (HEMS)*, Cocoa Beach, Florida, United States, 2022-09-26 - 2022-09-29. (LA-UR-22-29901)

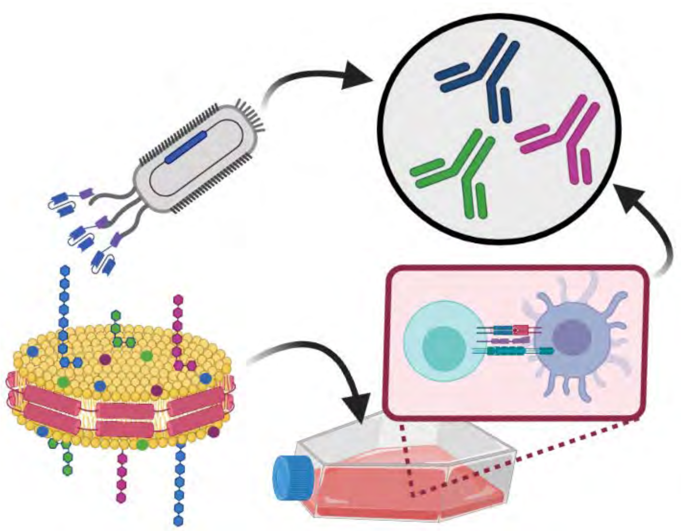
Posters

Sasiene, Z. J., W. S. Hlavacek, N. Velappan, E. S. LeBrun, N. H. Patterson, M. Dufresne, M. Farrow, J. Norris, R. Caprioli, T. G. Glaros and E. M. McBride. Multi-dimensional Portable Mass Spectrometry for Biological Detection. Presented at *Chemical and Biological Defense Science and Technology (CBD S&T) Conference*, San Francisco, California, United States, 2022-12-06 - 2022-12-09. (LA-UR-22-31362)

**Peer-reviewed*

Lipid Targeting for Select Agent Countermeasures

Jessica Kubicek-Sutherland
20220108ER



The unexpected nature of emerging and engineered pathogens requires broadly active medical countermeasures. LANL is identifying bacterial lipid targets to simultaneously select for broadly neutralizing therapeutic antibodies and to create cross-protective vaccines.

Project Description

The coronavirus (COVID-19) pandemic has highlighted gaps in our preparedness to combat novel threats. The unexpected nature of emerging and engineered pathogens requires broadly active medical countermeasures that can be administered immediately in order to minimize the impact on public health. The use of convalescent serum to treat COVID-19 patients shows the promise of neutralizing antibodies as first line therapeutics to combat novel threats. We are developing a novel pipeline to identify broadly neutralizing antibodies and then reverse engineer them to create cross-protective vaccine antigens. Traditionally, neutralizing antibodies and vaccines tend to target pathogen proteins but these molecules are prone to mutation and can be highly variable. Instead, we are targeting pathogen lipids which are conserved among bacterial classes and can therefore be used to provide a cross-protective response. In this project, we are simultaneously developing antibody therapeutics and a cross-protective vaccine to combat three Tier 1 bacterial select agent pathogens: Francisella tularensis, Burkholderia pseudomallei, and Yersini pestis.

Publications

Journal Articles

Kubicek-Sutherland, J. Z., P. A. Kocheril and M. I. Hiller. Evidence of excited-state lifetime enhancement in dimyristoyl-phosphocholine nanodiscs by ultraviolet absorption spectroscopy. 2023. *AIP Advances*. **13** (1): 015124. (LA-UR-22-25159 DOI: 10.1063/5.0102149)

Stromberg, L. R., M. M. Jones, A. Bitzer, S. Courtney, S. Jakhar, S. C. Moore, K. E. Klosterman, L. Lilley, Z. Stromberg, K. D. Lenz, J. Z. Kubicek-Sutherland and H. Mukundan. Understanding the Role of Amphiphilicity in Pathogen-Host Interactions during Innate Immunity: Gram-positive bacteria. Submitted to *Sage Journals*. (LA-UR-23-21585)

Stromberg, L., M. M. Jones, A. Bitzer, S. Courtney, S. Jakhar, S. C. Moore, K. E. Klosterman, M. I. Hiller, L. Lilley, Z. Stromberg, K. D. Lenz, J. Z. Kubicek-Sutherland and H. Mukundan. Understanding the Role of Amphiphilicity in Pathogen-Host Interactions during Innate Immunity: Gram-negative bacteria. Submitted to *Sage Journals*. (LA-UR-23-21975)

Stromberg, L., T. R. Llewellyn, M. M. Jones, A. Bitzer, S. Courtney, S. Jakhar, S. C. Moore, K. E. Klosterman, L. Lilley, Z. Stromberg, K. D. Lenz, J. Z. Kubicek-Sutherland and H. Mukundan. Understanding the Role of Amphiphilicity in Host-Pathogen Interactions During Innate Immunity: Gram-variable bacteria. Submitted to *Sage Journals*. (LA-UR-23-21970)

Velappan, N., F. Ferrara, S. D Angelo, D. Close, L. Naranjo, D. McCullogh, A. N. Gomez, M. Kedge and A. M. Bradbury. Direct selection of functional fluorescent-protein antibody fusions by yeast display. 2023. *PLOS ONE*. **18** (2): e0280930. (LA-UR-22-24741 DOI: 10.1371/journal.pone.0280930)

Presentation Slides

Kubicek-Sutherland, J. Z. Lipid Targeting For Broadly Active Bacterial Countermeasures. Presented at *DTRA CBDS&T Conference 2022*, San Francisco, California, United States, 2022-11-08 - 2022-11-08. (LA-UR-22-31491)

Velappan, N. Developing Antibodies to Viral Envelope Proteins: SARS CoV2 and Influenza A. Presented at *8th Annual International Conference on Biology*, Athens, Greece, 2022-06-20 - 2022-06-22. (LA-UR-22-25514)

Posters

Jacobsen, D. E., J. K. Banh, J. Z. Kubicek-Sutherland, K. D. Rector and R. Parchment. Whispering Gallery Mode Resonators as Labels for Biological Imaging. Presented at *Biophysical Society Annual Meeting*, San Diego, California, United States, 2023-02-18 - 2023-02-22. (LA-UR-23-21425)

Jones, M. M., M. I. Hiller and J. Z. Kubicek-Sutherland. Pseudomonas aeruginosa lipopolysaccharide presented in synthetic lipoprotein nanodiscs stimulates a robust immune response with reduced cytotoxicity. Presented at *American Society for Biochemistry and Molecular Biology*, Seattle, Washington, United States, 2023-03-24 - 2023-03-29. (LA-UR-23-22633)

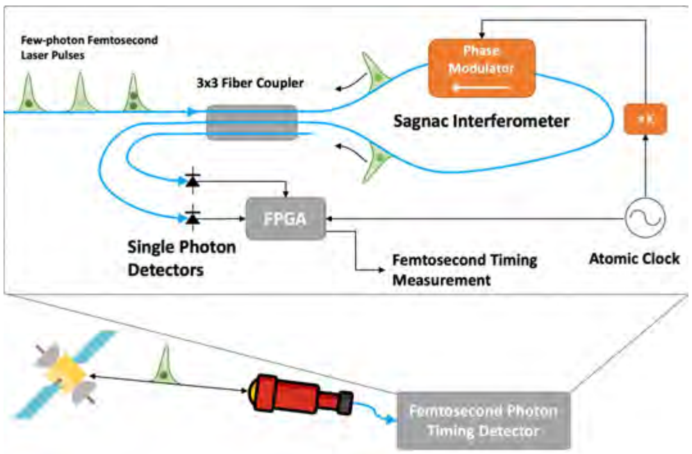
Lenz, K. D., M. Hiller, K. Klosterman, P. A. Kocheril, D. E. Jacobsen, S. Gnanakaran and J. Z. Kubicek-Sutherland. Nanodiscs as an anti-virulence therapeutic to treat bacterial infections. Presented at *IEEE Micro and Nanotechnology in Medicine*, Kapolei, Hawaii, United States, 2022-12-05 - 2022-12-09. (LA-UR-22-32174)

Velappan, N., S. C. Mozden, M. R. Bolding, S. Gnanakaran, D. P. Morales, M. E. Phipps, Z. Fox, Y. T. Lin, A. V. Zlotnik, G. S. Waldo, J. Z. Kubicek-Sutherland, H. T. B. Nguyen, R. K. Jha and A. M. Lillo. Developing Affinity Reagents for Novel Diagnostic Assays. Presented at *2022 Chemical and Biological Defense Science &Technology (CBD S&T) Conference*, San Franscisco, California, United States, 2022-12-05 - 2022-12-09. (LA-UR-22-31016)

**Peer-reviewed*

Few Photon Ultrafast Optical Timing Detection for Space Time Transfer

Jonathan Cox
20220130ER



Femtosecond precision time synchronization (a millionth of a billionth of a second) at the few photon level will enable numerous capabilities for national security, but existing single photon detectors are orders of magnitude less precise. The SPUD (single photon ultrafast detector) can achieve femtosecond precision time measurement by detecting the optical interference of each photon with itself. Novels algorithms running on a field-programmable gate array processor (FPGA) will measure the photon statistics to determine the time of arrival of femtosecond pulses with dramatically increased precision.

Project Description

Femtosecond (a millionth of a billionth of a second) precision time transfer to space will enable unprecedented new capabilities for remote sensing, signal collection, geolocation, space-based nuclear treaty verification and basic science. For comparison, the Global Positioning System (GPS) can only achieve meter positioning, in part, because it relies on radio frequency time transfer with ten nanosecond precision. However, the vast distances of space make such precision impossible without a quantum optical, femtosecond timing detector with few-photon sensitivity. The round-trip distance to the lowest satellites is over 250 miles, and 25,000 miles to GPS, so returning laser pulses will have at most a single photon. This project uses ultrafast laser technology, which generates femtosecond duration optical pulses, and the principles of quantum optics to measure the arrival time of photons with a precision hundreds of times more accurately than existing technology. As such, optical pulses can be bounced off of orbiting satellites, and returning photons timestamped with a precision far beyond that which is possible today. The project will develop and demonstrate a quantum optical, ultrafast timing detector in the lab and at range that can be integrated into United States space programs for intelligence or scientific benefit.

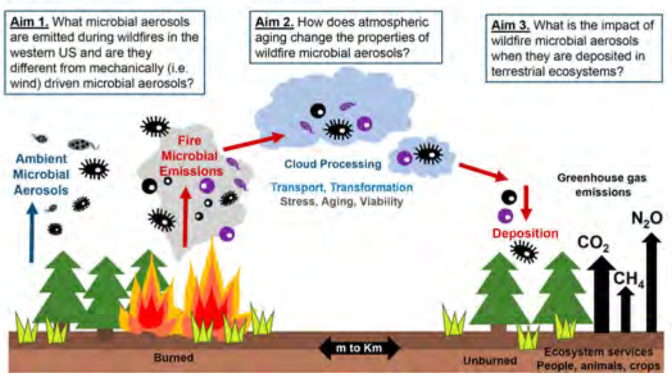
Science of Signatures

Exploratory Research
Continuing Project

Airborne Microbes from Wildfires: Direct Aerosol and Ecosystem Impacts and Human Health Implications

Katherine Benedict

20220183ER



There are many unanswered questions on the composition and prevalence of bioaerosol in the atmosphere. This image shows several atmospheric process related to bioaerosol which the project team will investigate. The team plans to focus on determining the importance of wildfire emitted biological aerosol and to specifically characterized the microbial composition and their viability once emitted. Additionally, the team will determine how they get transformed in the atmosphere and if it changes their ability to act as ice/cloud condensation nuclei. To determine the impacts when bioaerosol are deposited to downwind ecosystems we will perform controlled laboratory experiments.

Project Description

Current events have highlighted the potential for aerosols to carry infectious particles and broadly wildfire smoke is associated with negative health outcomes. Bioaerosols are a complex mixture of materials including living and dead microorganisms and are estimated to comprise a significant amount of atmospheric aerosol. Yet, bioaerosols emitted from wildfires have been the subject of limited research and a comprehensive characterization of bioaerosols currently does not exist, particularly the contribution from wildfires that are lofted and transported as smoke aerosol. The increase in wildfire activity across the western US underscores the urgency of addressing unanswered questions on the nature of bioaerosols to assess their impacts on humans, plants, soil health and climate. In this project we will conduct a series of laboratory and field experiments to begin to fill in these knowledge gaps. We will characterize the biology of the aerosol, how it changes with atmospheric transport, potential impacts on greenhouse gas emissions and ecosystems downwind, and the prevalence of human pathogens. This increased characterization of bioaerosol from smoke and their impact on processes in the Earth System will improve planning and impact assessments to forecast and model wildfire smoke's effects on ecosystems and human health.

Publications

Presentation Slides

Benedict, K. B., A. S. M. Shawon, K. J. Gorkowski, J. E. Lee, A. C. Aiken, M. K. Dubey, M. E. Kroeger and A. Gutierrez. Smoke Properties from Laboratory Burns. . (LA-UR-23-20051)

Benedict, K. B., M. E. Kroeger and M. B. N. Albright. Airborne Microbes from Wildfires: Direct Aerosol and Ecosystem Impacts and Human Health Implications. . (LA-UR-21-30937)

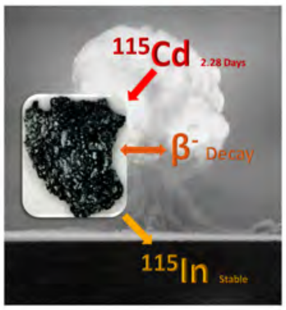
Dale, T. T. Bio-based solutions to transform the climate and clean energy systems. . (LA-UR-22-32234)

Kroeger, M. E. Structure-to-Function: Microbial Dynamics of Disturbed and Natural Ecosystems. . (LA-UR-23-20005)

**Peer-reviewed*

Indium Isotopic Ratios: A New Measurement for the Nuclear Forensics Toolbox

Daniel Meininger
20220259ER



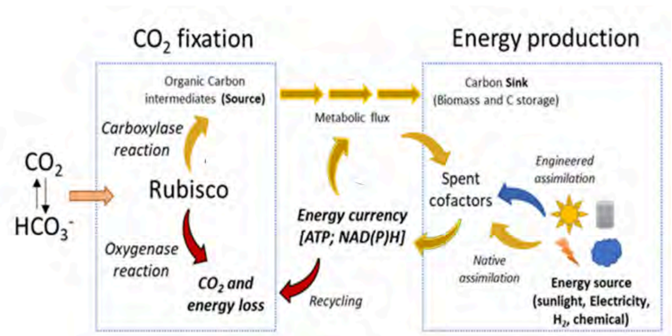
The short-lived fission product 115Cd (Cadmium) produced during nuclear fission is an essential diagnostic signature for post-detonation nuclear forensics. 115Cd, with a 2.2 day half-life, undergoes beta decay to form the stable 115In (Indium) daughter. By measuring the perturbed isotopic ratio of 115In/113In and the total concentration of In in nuclear debris, the amount of 115Cd originally present in a sample that was produced as a result of nuclear fission can be determined. This capability will extend the analysis timeline for this fission decay chain.

Project Description

Measurements of fission products (radioactive elements produced as a result of nuclear fission) provide key analytical insights into nuclear events. However, many of these essential diagnostic signatures produced as a result of nuclear fission are short lived and as time passes they decay away and can no longer be measured. As these fission products decay into different stable elements, they perturb the natural isotopic ratios of these elements into which they decay. In some cases this perturbation can be measured and information regarding the long decayed away fission product can be obtained. This work will demonstrate the ability to measure one of these vitally important short lived fissions products, cadmium isotope 115, in old nuclear debris through high precision isotopic measurements of the stable daughter isotope of indium 115. This type of advance in fission product analysis allows for the examination of a nuclear event years beyond the traditional timeline and allows for necessary re-examination of the US nuclear stockpile.

Carbon Dioxide (CO2) Fixation Facilitated by Energy Equilibrium

Cesar Gonzalez Esquer
20220387ER



CO2 fixation by Rubisco is dependent on a pool of energy cofactors that drive the carbon flux from the carbon source (site of CO2 fixation) to the sink (biomass and bioproducts). In this project, the team aims to improve both CO2 fixation and metabolic flux into carbon sinks, by supplementing the microbial platforms with nutrients and by genetically engineering new CO2 fixation mechanisms.

Project Description

Many essential industries in the United States greatly rely on the burning of non-renewable fuels, consequently releasing greenhouse gases −specifically carbon dioxide (CO2)− into the atmosphere. This excess of CO2 is a main contributing factor to the extreme fluctuations in Earth's climate, which in turn affects crop productivity, weather patterns, and ecosystem equilibria, resulting a high economic impact when mitigating these adverse effects. We seek to leverage autotrophic metabolism (microbial mechanisms that utilize sunlight/chemicals as energy sources for the synthesis of organic carbon molecules) as a platform for large-scale CO2 recovery and its bioconversion into valuable commodity chemicals. For this purpose, we follow two strategies: i) enhancing the native CO2 fixation mechanisms by characterizing the effects of feeding reduced molecules on growth rate and carbon storage in microbial biomass and ii) genetically engineering non-native CO2 fixation pathways with improved efficiency under industrially-relevant conditions (targeting high product yields). Success will advance the incorporation of biotechnological platforms into the existing bioeconomy, reduce the Nation's dependence on foreign resources, assist in the compliance of policy and regulation for CO2 release mitigation in industrial processes and address climate effects due to the accumulation of CO2 in the atmosphere.

Publications

Journal Articles

Trettel, D. S., C. A. Neale, S. Gnanakaran and C. R. Gonzalez Esquer. Monatomic Ions Influence Substrate Permeation Across Bacterial Microcompartment Shells. Submitted to *Scientific Reports*. (LA-UR-23-20029)

Presentation Slides

Gonzalez Esquer, C. R. From CO2\xc2\xa0Fixation to Renewable Chemical Production in Photosynthetic Platforms. . (LA-UR-22-20666)

Gonzalez Esquer, C. R. Reconfiguring photosynthetic microbes for their development as biotechnological platforms. . (LA-UR-23-21260)

Pacheco, S. L. and C. R. Gonzalez Esquer. Engineering of the Synecchocystis CO2 -concentrating mechanism. . (LA-UR-22-32528)

Trettel, D. S. How I became fixated on BMCs, and what I learned along the way. Presented at *Kerfeld lab retreat at Asilomar*, Pacific Grove, California, United States, 2023-02-07 - 2023-02-09. (LA-UR-23-21089)

Posters

Pacheco, S. L. and C. R. Gonzalez Esquer. Characterization of a modified carbon fixation mechanism in Synechocystis sp PCC 6803. Presented at *New Mexico Research Symposium*, Albuquerque, New Mexico, United States, 2022-11-05 - 2022-11-05. (LA-UR-22-31713)

Trettel, D. S., C. A. Neale, S. Gnanakaran and C. R. Gonzalez Esquer. Monatomic ions influence substrate permeation across bacterial microcompartment shells. Presented at *ASBMB 2023 American Society for Biochemistry and Molecular Biology*, Seattle, Washington, United States, 2023-03-25 - 2023-03-28. (LA-UR-23-22325)

**Peer-reviewed*

Dynamic Coalition Management in Multi-Agent Sensor Networks

Przemyslaw Wozniak
20220392ER

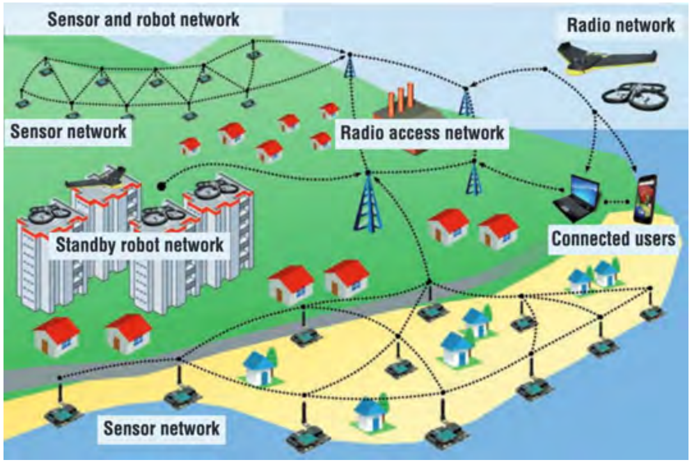


Illustration of the Multi-Agent Sensor Network concept applied to disaster recovery (from Erdelj et al. 2017, Pervasive Computing 17, 1536). In order to succeed, modern heterogeneous sensor networks must integrate diverse government, commercial, academic, and international assets. Dynamic Coalition Architecture offers a decentralized approach to coordinate autonomous agents that form temporary coalitions to perform efficient data collections. However, a suitable optimization approach is lacking. Robust optimization (RO) combined with rolling horizon (RH) estimation can provide an optimal, near real-time solution that will satisfy all problem constraints for all possible realizations of the unknown parameters as a way of hedging against the risk.

Project Description

A revolution in surveillance technology is taking place at the intersection of Artificial Intelligence (AI) and the Internet of Things (IoT). Next generation surveillance systems will deploy networks of intelligent agents acting in the environment, requiring a mix of collaborative and individual behavior to accomplish their mission. While numerous approaches are being explored, this project will advance a long-term vision that can address often unique challenges posed by national security problems and government applications. The project will develop an event-driven framework to address the main barriers to wider adoption by optimizing the underlying complex resource management problem, while providing probabilistic guarantees under uncertainty. This new high impact capability will be demonstrated in the context of space surveillance using telescope networks and physical security with drone fleets, two areas of urgent national needs representing a large class of real-world problems. The solution goes beyond the limits of strict command-and-control to mitigate multi-level security issues and agency stovepipes that so often impede timely government response. This new approach is expected to strongly impact a wide range of applications, including physical security, emergency response, industrial/ environmental monitoring, nuclear non-proliferation, and space sciences.

Publications

Presentation Slides

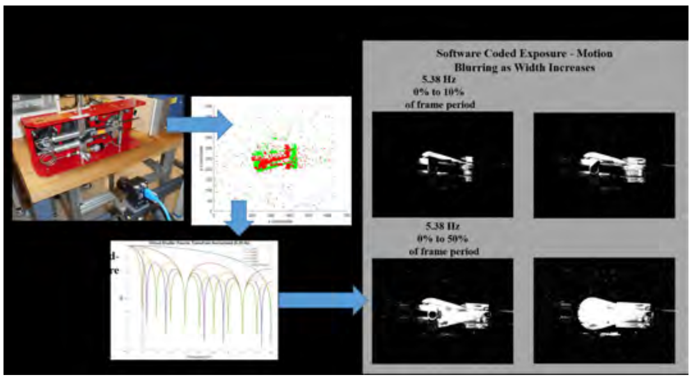
Riabova, S. and H. L. Hijazi. Multi-agent Optimization for Space Situational Awareness. Presented at *T division lightning talk student symposium*, Los Alamos, New Mexico, United States, 2022-08-09 - 2022-08-10. (LA-UR-22-28316)

Wozniak, P. R. and S. Riabova. Optimizing Space Traffic Management. . (LA-UR-22-26126)

**Peer-reviewed*

Event-Driven Imagers for Capturing Light Field Video

David Mascarenas
20220426ER



A concept for a neuromorphic light-field imager that is low-power, low-latency and has a high dynamic range and leverages coded-exposure techniques for a shutter speed that can be varied in post-processing.

Project Description

The goal of this work is to develop an event-based computational imager for capturing time-varying four-dimensional (4D) light fields that contain information on the direction at which light rays are entering an imager for a defined volume. The development of an event-based light field imager coupled with advances made by the team in the area of digital coded exposures would allow for the generation of images where the focus/depth-of-field and shutter could be modified in post processing. As a result, the proposed imager would generate data such that focus/depth-of-field and shutter speed/exposure could effectively be changed in post-processing when forming frames. The development of an event-based light-field imager would also allow for the measurement of depth. Event-based imagers are known to have high dynamic range (~120 decibels) and to be able to capture high-speed phenomena at low power with low memory/bandwidth requirements. By leveraging the advantages of event-based imagers for the purpose of capturing time-varying 4D light-fields, coupled with coded exposure technology, the team will be able to create a new type of computational imager that could be used for a wide variety of Los Alamos National Laboratory applications such as monitoring manufacturing processes, remote sensing, unattended monitoring, synthetic aperture imaging, robotics and microscopy.

Publications

Conference Papers

Green, A. W., M. F. Mello da Silva, A. Cattaneo and D. D. L. Mascarenas. Digital Coded Exposure for Physically-Motivated, Event-Based Frame Formation, Interpolation and Motion Blur Control. Presented at *CVPR 2023 - 4th International Workshop on Event-based Vision.* (Vancouver, Canada, 2023-06-19 - 2023-06-19). (LA-UR-23-22820)

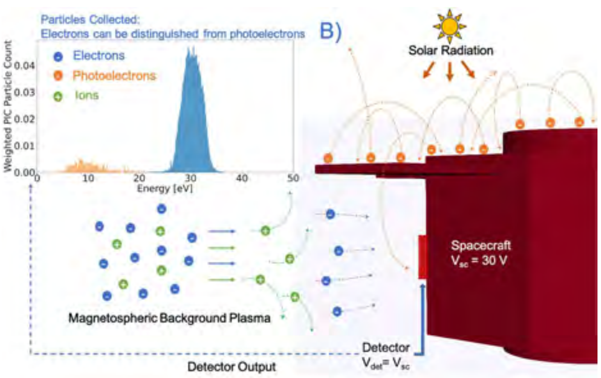
Presentation Slides

Green, A. W., P. Meyerhofer, A. Cattaneo and D. D. L. Mascarenas. Digital Image Correlation Using an Event-Driven Silicon Retina. Presented at *International Modal Analysis Conference (IMAC)*, Orlando, Florida, United States, 2022-02-07 - 2022-02-10. (LA-UR-22-20038)

**Peer-reviewed*

Enabling Cold-Electron Measurements and New Space Missions

Carlos Maldonado
20220453ER



A challenge addressed by this research is to distinguish the signals of spacecraft-generated photoelectrons and magnetospheric electrons in the detector. The team propose to accomplish this by varying the voltage of the spacecraft relative to the ambient magnetosphere (via emission of an electron beam) since this will (i) not change the appearance of the spacecraft generated photoelectrons as seen by the detector but will (ii) strongly vary the appearance of the magnetospheric electrons. Thus, by varying the spacecraft potential, the small population of magnetospheric electrons can be distinguished from the very large population of photoelectrons.

Project Description

This project taps into Los Alamos National Laboratory multidisciplinary strengths and further develops its capabilities by conducting laboratory experiments to test and validate novel techniques required to measure low-energy (i.e. cold) magnetospheric plasma. The controlled plasma environment created in a ground-based facility will allow for the photoelectron and ambient plasma populations to be separated and measured using differential biasing techniques. These measurements will then be used to validate computational models which can then be extended to explore and estimate the use of these techniques for space-based applications. Space missions are critical to maintain Los Alamos' innovation and vitality, excellence in the community and to support the national security mission. Enabling cold-plasma measurements (and possibly future cold-plasma missions) also supports Los Alamos' ability to respond to threats in space since understanding the space environment is critical to protect space and ground-based assets. For instance, the cold plasma properties might be critical to the efficiency of radiation belt remediation schemes that must protect the country from the catastrophic consequences of a high-altitude nuclear explosion.

Publications

Journal Articles

Maldonado, C. A., P. A. Resendiz Lira, G. L. Delzanno, B. A. Larsen, D. B. Reisenfeld and V. Coffey. A review of instrument techniques to measure magnetospheric cold electrons and ions. 2023. *Frontiers in Astronomy and Space Sciences*. **9**: 1005845. (LA-UR-22-25055 DOI: 10.3389/fspas.2022.1005845)

Ripoll, J. F., V. Pierrard, G. S. Cunningham, X. Chu, K. Sorathia, D. Hartley, S. Thaller, V. G. Merkin, G. L. Delzanno, S. De Pascuale and A. Y. Ukhorskiy. Modeling of the electron plasma density for radiation belt physics. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-22-32601)

Conference Papers

Resendiz Lira, P. A., G. L. Delzanno, C. A. Maldonado and J. E. Borovsky. Modeling of Cold Electron Measurements in the Magnetosphere using active spacecraft potential control.. Presented at *AGU Fall 2021*. (New Orleands, Louisiana, United States, 2021-12-13 - 2021-12-17). (LA-UR-21-31980)

Reports

Delzanno, G. L., J. E. Borovsky, J. Bortnik, C. R. Chappell, P. A. Fernandes, D. Gallagher, J. Goldstein, M. G. Henderson, J. C. Holmes, G. B. Hospodarsky, V. K. Jordanova, C. A. Maldonado, Y. Nishimura, D. B. Reisenfeld, V. Roytershteyn, R. M. Skoug, E. Spanswick, M. Usanova, E. Donovan, P. A. Resendiz Lira, O. Koshkarov and D. Svyatsky. The Need to Understand the Cold Ion and Cold Electron Populations of the Earth's Magnetosphere:. Unpublished report. (LA-UR-22-27269)

Maldonado, C. A., G. L. Delzanno, P. A. Resendiz Lira, J. H. Lee, B. A. Larsen, P. A. Fernandes, G. R. Wilson, D. B. Reisenfeld, J. E. Borovsky, J. Goldstein, V. Coffey, D. Gallagher, N. Kitamura and C. R. Chappell. The Critical Need for Innovations in Instruments and Techniques to Enable In-Situ Cold Ion and Cold Electron Measurements within the Magnetosphere. Unpublished report. (LA-UR-22-30409)

Presentation Slides

Delzanno, G. L. IMPPACT: Invisible Magnetospheric Plasma Pathfinder with Active Charging Techniques. . (LA-UR-22-29117)

Delzanno, G. L. IMPPACT: Invisible Magnetospheric Plasma Pathfinder with Active Charging Techniques. . (LA-CP-22-20663)

Delzanno, G. L. IMPPACT: Invisible Magnetospheric Plasma Pathfinder with Active Charging Techniques. . (LA-CP-22-20671)

Resendiz Lira, P. A., G. L. Delzanno, J. E. Borovsky and C. A. Maldonado. Active Spacecraft Potential Control with an Electron Beam to Enable Cold Electron Measurements in the Earth's Magnetosphere. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32818)

Resendiz Lira, P. A., G. L. Delzanno, J. E. Borovsky and C. A. Maldonado. Cold-Plasma Measurements in the Earth's Magnetosphere. Presented at *National Radio Science Meeting*, Boulder, Colorado, United States, 2023-01-10 - 2023-01-14. (LA-UR-22-33177)

Resendiz Lira, P. A. and D. Svyatsky. Cold electron measurements with active S/C potential control. . (LA-UR-23-23113)

Maldonado, C. A., G. L. Delzanno, P. A. Resendiz Lira, B. A. Larsen, D. B. Reisenfeld, J. Goldstein, D. Gallagher, G. R. Wilson, C. R. Chappell, J. E. Borovsky, N. Kitamura and J. H. Lee. The Need for Innovations in Instruments and Techniques to Enable Cold Ion and Cold Electron Measurements within the Magnetosphere. Presented at *GEM Summer Workshop*, Honolulu, Hawaii, United States, 2022-06-20 - 2022-06-24. (LA-UR-22-30408)

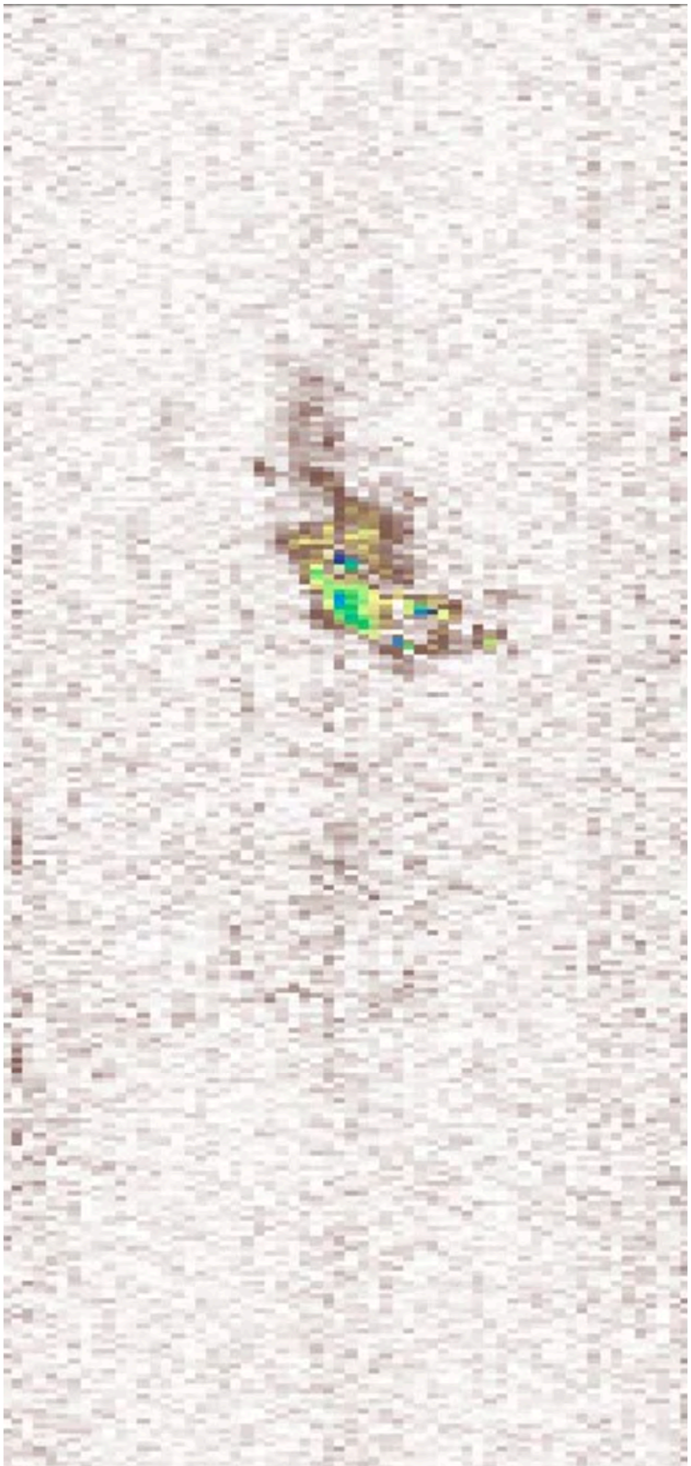
Posters

Resendiz Lira, P. A., G. L. Delzanno, J. E. Borovsky and C. A. Maldonado. Active Spacecraft Potential Control with an Electron Beam to Enable Cold Electron Measurements in the Earth's Magnetosphere. Presented at *GEM Summer Workshop*, Honolulu, Hawaii, United States, 2022-06-19 - 2022-06-24. (LA-UR-22-25659)

**Peer-reviewed*

High Resolution Atmospheric Chemistry Mapping by Coordinated Space- and Ground-Based Hyperspectral Imaging

Steven Love
20220463ER



The new NACHOS instrument condenses a full hyperspectral imager, devices typically only deployable on massive and expensive platforms,into the agile and compact CubeSat geometry. These ultra-compact instruments (both satellite- and ground-based) will compile 2D spectral images, acquired while sweeping out one of the spatial dimensions, into a full hyperspectral datacube. On-board matched filter processing will condense the datacubes into two-dimensional density maps, enabling download from the bandwidth limited CubeSat. The unprecedented spatio-temporal resolution of these maps will reveal the fine-grained detail of gases relevant to topics spanning global warming, human health and Earth science.

Project Description

The proposed work, which would be, to our knowledge, the first-ever square-shaped miniature satellite (CubeSat)-based hyperspectral imaging gas-sensing science campaign, represents a crucial step toward a long-term vision where inexpensive small-satellite constellations complement, and perhaps eventually supplant, traditional large-satellite-based instruments. As such, this project aims to demonstrate that our ultra-miniaturized instrument is competitive with, or even exceeds traditional large-satellite instruments in chemical detection applications. If successful, this proposed work could herald a new approach to Deparment of Energy(DOE)/National Nuclear Security Administration (NNSA) missions, where constellations of agile, inexpensive CubeSat-based instruments are deployed with features tailored for specific detection objectives, providing global atmospheric monitoring at nearly real-time speeds. Potentially, these constellations could employ an inter-satellite tipping and queueing scheme, where one satellite detects an anomalous event, then signals other satellites with different capabilities (e.g. increased spatial resolution, different spectral range) to identify the cause, and if it is relevant to DOE/NNSA missions; an arrangement that would provide immediate clarity, whereas data download and processing in current monitoring produces a significant delay between detection and classification.

Publications

Journal Articles

Theiler, J. P. Homeopathic priors?. Submitted to *arXiv*. (LA-UR-22-32575)

Theiler, J. P. and S. Matteoli. Bayesian Target Detection Algorithms for Solid Subpixel Targets in Hyperspectral Images. Submitted to *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-23-22409)

Conference Papers

Love, S. P., K. Post, L. A. Ott, M. E. Dale, C. L. Safi, K. G. Boyd, H. D. Mohr, C. R. Ward, M. P. Caffrey, J. P. Theiler, B. R. Foy, M. P. Hehlen, C. G. Peterson, R. L. Hemphill, J. Wren, A. A. Guthrie, N. Dallmann, P. S. Stein, A. G. Meyer and M. K. Dubey. NACHOS, a CubeSat-based high-resolution UV-Visible hyperspectral imager for remote sensing of trace gases: System overview, science objectives, and preliminary results. Presented at *Small Satellite Conference*. (Logan, Utah, United States, 2022-08-06 - 2022-08-11). (LA-UR-22-25287)

Theiler, J. P. Bayesian vs generalized likelihood ratio detection of solid sub-pixel targets. Presented at *International Geoscience and Remotes Sensing Symposium (IGARSS)*. (Padadena, California, United States, 2023-07-16 - 2023-07-21). (LA-UR-23-20197)

Theiler, J. P. Anisotropic background models for spectral target detection. Presented at *International Society for Optics and Photonics (SPIE) Defense and Commercial Sensing Conference*. (Orlando, Florida, United States, 2023-04-30 - 2023-05-04). (LA-UR-23-23325)

Theiler, J. P. and C. X. Ren. Iterative R&R (Rotation and Remarginalization) for Detecting Targets in Spectral Imagery. Presented at *International Society for Optics and Photonics (SPIE) Optics and Photonics Conference*. (San Diego, California, United States, 2022-08-22 - 2022-08-24). (LA-UR-22-28002)

Presentation Slides

Love, S. P., K. Post, L. A. Ott, M. E. Dale, C. L. Safi, K. G. Boyd, H. D. Mohr, C. R. Ward, M. P. Caffrey, J. P. Theiler, B. R. Foy, M. P. Hehlen, C. G. Peterson, R. L. Hemphill, J. Wren, A. A. Guthrie, N. Dallmann, P. S. Stein, A. G. Meyer and M. K. Dubey. NACHOS, a CubeSat-based high-resolution UV-Visible hyperspectral imager for remote sensing of trace gases: System overview, science objectives, and preliminary results. Presented at *Small Satellite Conference*, Logan, Utah, United States, 2022-08-06 - 2022-08-11. (LA-UR-22-28181)

Post, K. Terahertz spectroscopy of high temperature superconductors in pulsed magnetic fields. Presented at *Job Talk*, San Diego, California, United States, 2022-07-29 - 2022-07-29. (LA-UR-22-27441)

Post, K., L. A. Ott, M. E. Dale, C. L. Safi, K. G. Boyd, H. D. Mohr, J. P. Theiler, B. R. Foy, M. P. Hehlen, C. R. Ward, M. P. Caffrey, R. L. Hemphill, M. K. Dubey and S. P. Love. The NACHOS CubeSat-Based Hyperspectral Imager: Laboratory Characterization and On-Earth Deployment. Presented at *Smallsat*, Logan, Utah, United States, 2022-08-06 - 2022-08-11. (LA-UR-22-27301)

Theiler, J. P. and C. X. Ren. Iterative R&R for detecting targets in spectral imagery. Presented at *International Society for Optics and Photonics (SPIE) Optics and Photonics Conference*, San Diego, California, United States, 2022-08-21 - 2022-08-24. (LA-UR-22-28559)

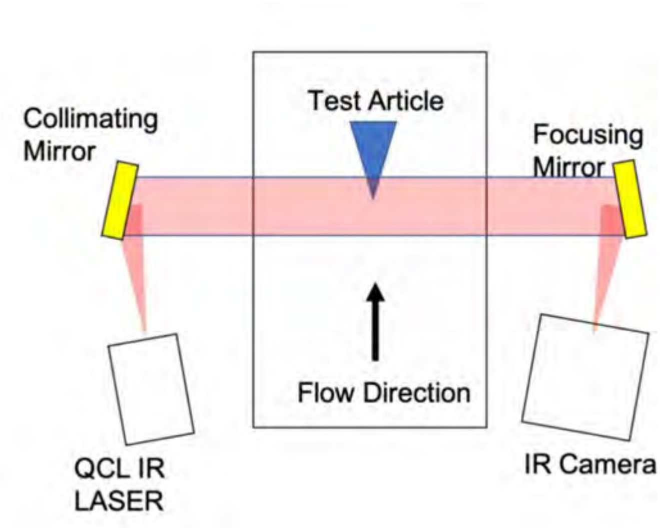
Posters

Theiler, J. P. Bayesian oddities: homeopathic priors and inadmissible detectors. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2023-03-07 - 2023-03-09. (LA-UR-23-20572)

**Peer-reviewed*

Precision Measurement of Signatures of Hypersonic Flight

John Bowlan
20220734ER



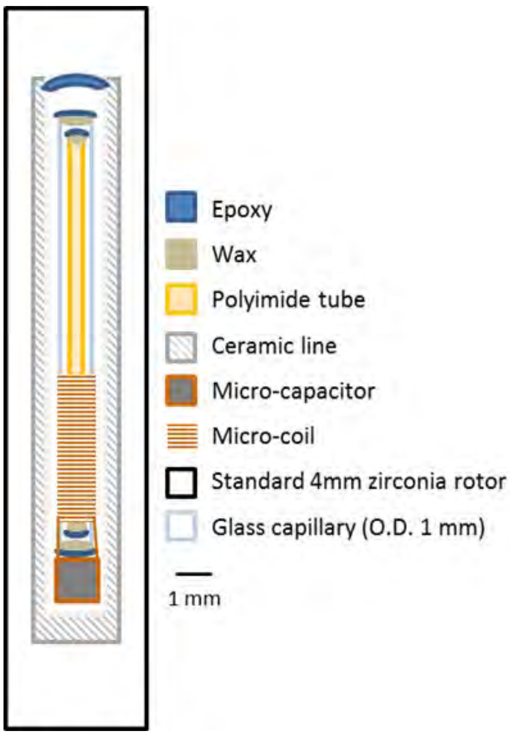
The purpose of this project is to apply chemical imaging to flow fields. The basic principle of the measurement is that the test article and flow are illuminated by a collimated beam of laser light through windows in the wind tunnel. The target is then re-imaged onto an infrared camera. The laser light is tuned to an absorption resonance of a particular gas species. When the gas species is present, the absorption makes the pixel appear dark.

Project Description

This project directly addresses the high priority national security mission to develop better methods for detecting and understanding the signatures of hypersonic flight. There is a current high priority need in the government to better understand the infrared/optical signatures of hypersonic flight vehicles to improve remote detection and tracking capabilities. The infrared/optical signature depends on emission by the vehicle, as well as the hot gas species in the flow surrounding the vehicle. The objective of this seedling proposal is to develop novel methods to precisely quantify the chemical effects which take place in hypersonic flow, and how this chemistry affects the optical signature.

Employing Magic Angle Coil Spinning (MACS) as a Method for Analyzing Radioactive Samples with Solid-State Nuclear Magnetic Resonance Spectroscopy

Harris Mason
20220735ER



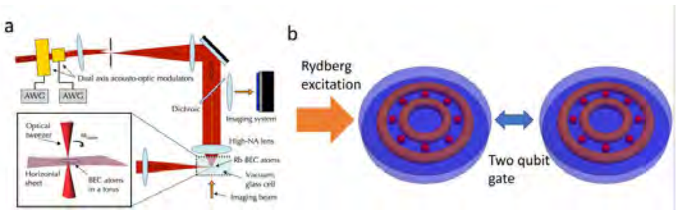
A proposed design for a MACS sample container for use in MAS NMR. This design is for a 4 millimeter (outer diameter) rotor but is easily adapted for other configurations.

Project Description

Hazardous materials are a fact of life for many of the missions at Los Alamos National Laboratory. Radioactive, toxic, and explosive materials are routinely investigated as a part of many of the activities occurring at the lab. As such, we need methods that can investigate and understand the complex chemistry of these materials. In many cases, we need to understand how these materials behave in their native solid state. Solid-state Nuclear Magnetic Resonance (NMR) is a useful method for investigating these materials, but is hindered by the need to safely encapsulate these materials during analysis. The encapsulation reduces the amount of material needed and makes the experiment safer, but at the expense of the time needed to collect data. The method we propose, magic angle coil spinning (MACS), allows us to both encapsulate the material and provide signal enhancement. We will develop a MACS system with an eye to studying radioactive materials and will enable us to pursue unique radiochemical experiments including 239 Plutonium (Pu) NMR.

Atomic Ensemble Qubits with a Strongly Interacting One Dimensional Gas of Atoms

Kevin Henderson
20220760ER



This image demonstrates the basic schematic of the core technology to create an atomic ensemble qubit and demonstrate a two-qubit gate. The first image shows the painted potential setup to realize various ring trap configurations for the gate operation. The second image shows a possible schematic of the two-qubit gate.

Project Description

Quantum computation is one of the most transformative technologies for many critical applications. Developing a novel scheme of ensemble qubits will be perfectly aligned with the priority of quantum information science in Los Alamos National Laboratory (LANL) and the National Quantum Initiative. Although software development is important in finding useful applications, there is still an urgent need to find the best technology for quantum computing hardware. Demonstrating ensemble qubits with a long coherence time and high gate fidelity will allow LANL to lead the atom-based quantum hardware development.

Early Detection of Explosive Volcanic Eruptions Using Very High Frequency (VHF) Radiation from Vent Discharges

Sonja Behnke
20190107ER

Electrical activity during explosive volcanic eruptions can be detected using instruments designed to detect radio waves in the very high frequency range (VHF), as depicted here. At the onset of an explosive event, meter-scale "vent discharges" occur in intense bursts at the vent of a volcano. They produce a characteristic VHF signature that can be used to identify when explosive eruptions occur. The LDRD team devised a method for automated detection of explosive volcanic eruptions by exploiting this signature. This new technique provides a reliable means to quickly detect and characterize eruptions from remote, high-risk volcanoes that threaten air traffic.

Project Description

Volcanic ash from an explosive volcanic eruption can rise to aircraft cruising altitudes within 5 minutes of eruption onset, posing a serious threat to aircraft. Thus, timely detection of explosive eruptions and rapid characterization of the resulting ash cloud is a priority for volcano observatories in the United States. The goals of this project are to identify the signal characteristics of a class of volcanic lightning discharges (“vent discharges”) that commonly occur in ash plumes and determine how to exploit these characteristics in a radio frequency-based volcanic eruption monitoring system. This work will advance the state of the art of volcano monitoring and address gaps in current methods. In addition, the knowledge gained about the signal characteristics of vent discharges and the methods to discriminate them from other types of lightning and other radio frequency transients can be applied to mission areas that are of interest to the National Counter Proliferation Center. For example, vent discharges are similar to electrical discharges produced by chemical explosions; the scientific understanding gained from this work can help inform a science-based simulation framework to model the characteristics and signatures of a non-nuclear test device, from early detonation to late time combustion.

Technical Outcomes

The project successfully completed its goals to identify the signal characteristics of vent discharges and to determine how to use these characteristics in volcano monitoring. The team created a logistic regression model that can accurately predict whether a radio frequency impulse is part of a flash or a period of vent discharges. This result was used to demonstrate how the logistic regression model could be used in a novel, machine-learning eruption detection algorithm.

Publications

Journal Articles

. E. H. *. S. S. *. I. M. *. M. D. Behnke, S. A. and S. A. Behnke. Radio Frequency Characteristics of Volcanic Lightning and Vent Discharges. 2021. *Journal of Geophysical Research: Atmospheres*. **126 (18): e2020JD034495. (LA-UR-20-30282 DOI: 10.1029/2020JD034495)

*Behnke, S. A., H. E. Edens, J. Theiler, D. J. Swanson, S. Senay, A. R. Van Eaton, M. Iguchi and D. Miki. Discriminating Types of Volcanic Electrical Activity: Toward an Eruption Detection Algorithm. 2022. *Geophysical Research Letters*. **49** (15): e2022GL099370. (LA-UR-21-29317 DOI: 10.1029/2022GL099370)

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*Cimarelli, C., S. Behnke, K. Genareau, J. M. Harper and A. R. Van Eaton. Volcanic electrification: recent advances and future perspectives. 2022. *Bulletin of Volcanology*. **84** (8): 78. (LA-UR-22-26701 DOI: 10.1007/s00445-022-01591-3)

Van Eaton, A. R., J. Lapierre, S. A. Behnke, C. Vagasky, C. J. Schultz, M. Pavolonis, K. Bedka and K. Khlopenkov. Lightning rings and gravity waves: Insights into the giant eruption plume from Tonga's Hunga Volcano on 15 January 2022. Submitted to *Geophysical Research Letters*. (LA-UR-23-23258)

*B. S. *. E. H. *. T. R. Haley, S. *., S. Haley and S. Behnke. Observations Show Charge Density of Volcanic Plumes is Higher Than Thunderstorms. 2021. *Journal of Geophysical Research: Atmospheres*. **126** (19): e2021JD035404. (LA-UR-21-25344 DOI: 10.1029/2021JD035404)

Presentation Slides

Behnke, S. A. Volcanic Plume Electrification and Lightning. . (LA-UR-22-23470)

Behnke, S. A. EGU22-2972: Using radio frequency signal classification to monitor explosive eruptive activity. Presented at *European Geosciences Union General Assembly*, Vienna, Austria, 2022-05-23 - 2022-05-27. (LA-UR-22-24732)

Behnke, S. A. Volcanic Lightning: The Electrical Charging and Discharging of Volcanic Eruption Plumes. Presented at *IEEE 14th Annual EOS/ESD Symposium*, Reno, Nevada, United States, 2022-09-18 - 2022-09-18. (LA-UR-22-28319)

Behnke, S. A., H. E. Edens, J. P. Theiler, D. J. Swanson, S. Senay, M. Iguchi and D. Miki. A Method for Discriminating Types of Volcanic Electrical Activity. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31924)

Behnke, S. A., H. E. Edens, J. P. Theiler, D. J. Swanson, S. Senay, M. Iguchi and D. Miki. Using Radio Frequency Measurements of Volcanic Electrical Activity for Volcanic Eruption Detection. . (LA-UR-22-26236)

Behnke, S. A., H. E. Edens, J. P. Theiler, D. J. Swanson, S. Senay, M. Iguchi and D. Miki. Applying machine learning methods to detect explosive volcanic eruptions with volcanic lightning observations. Presented at *IAVCEI 2023 Scientific Assembly*, Rotorua, New Zealand, 2023-01-30 - 2023-01-30. (LA-UR-23-20253)

Posters

Behnke, S. A., H. E. Edens, S. Senay, J. B. Johnson, K. B. Eack, M. P. Caffrey, J. P. Theiler, A. R. Van Eaton, D. J. Schneider, M. Iguchi and D. Miki. Early Detection of Explosive Volcanic Eruptions Using VHF Radiation from Vent Discharges. Presented at *American Geophysical Union Fall Meeting 2019*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32189)

Behnke, S. A., H. E. Edens and J. P. Theiler. Vent Discharges Produced by Explosive Volcanic Eruptions: Characteristics, Signatures, and Volcano Monitoring Applications. Presented at *American Geophysical Union Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31441)

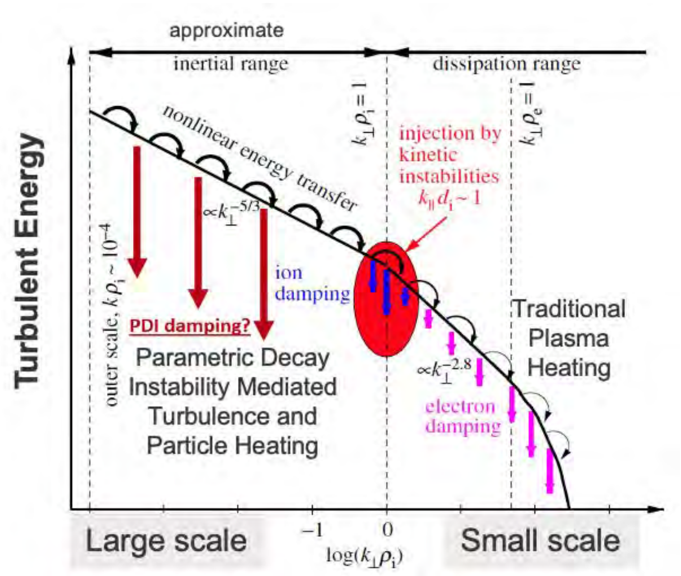
Haley, S. L., S. A. Behnke, H. E. Edens and R. J. Thomas. Exploring Properties of Volcanic Lightning using Electric Field Change Measurements and 3D Lightning Mapping Data. Presented at *American Geophysical Union Fall Meeting 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29374)

Swanson, D. J., S. A. Behnke, C. M. Smith and A. R. Van Eaton. Examining the Relationship Between Electrical Activity and Jet Velocity During Explosive Volcanic Eruptions at Sakurajima Volcano. Presented at *American Geophysical Union Fall Meeting 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29343)

**Peer-reviewed*

Unveiling the Heating and Acceleration of Solar Wind by "Touching" the Sun with the Parker Solar Probe

John Steinberg
20200270ER



Solar wind flow and magnetic field exhibit turbulence with a broad spectrum spanning several decades, essential for plasma heating in the solar wind. While traditional models focused on the dissipation of turbulence at small scales, this work has also identified new turbulence generation and plasma heating processes at large scales, mediated by the parametric decay instabilities of Alfven waves. The Parker Solar Probe satellite is providing unique in-situ measurements to test our theoretical modeling.

Project Description

This project aims at understanding the origin of Solar Wind (SW), a plasma gas that is heated and accelerated away from the Sun and fills the solar system. This is a fundamental question for understanding of the space weather and it could have a major impact on understanding how SW impacts Earth's nearby space environment known as the magnetosphere. This project brings together observations, data analysis, theory, and numerical modeling of SW plasma particles and magnetic fields. It builds capabilities in space plasma and field detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Technical Outcomes

A new fundamental understanding of properties of compressible turbulence in near-sun solar wind observed by Parker Solar Probe was achieved. Density fluctuations were found to be important and to increase linearly with turbulence amplitude, both in observations and magnetohydrodynamic plasma simulations. New tools developed to differentiate wave modes in the simulations showed the dominant density fluctuations are best described as low-frequency nonlinear structures rather than compressible waves. Density structures result from strongly driven turbulence.

Publications

Journal Articles

*Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. T. Dahlin and Q. Zhang. Slow Shock Formation Upstream of Reconnecting Current Sheets. 2022. *The Astrophysical Journal*. **926** (1): 24. (LA-UR-21-27254 DOI: 10.3847/1538-4357/ac423b)

Broll, J. M., J. T. Steinberg and E. K. Conrad. Identifying spectral indices and breakpoints in space1 plasma measurements. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-22-30132)

Du, S., H. Li, X. Fu, Z. Gan and S. Li. Magnetic Energy Conversion in MHD: Curvature Relaxation and Perpendicular Expansion of Magnetic Fields. Submitted to *Astrophysical Journal*. (LA-UR-21-30494)

Du, S., H. Li, X. Fu and Z. Gan. Anisotropic energy transfer and conversion in magnetized compressible turbulence. Submitted to *Astrophysical Journal*. (LA-UR-23-20686)

Du, S., H. Li and F. Guo. Onset of magnetic reconnection at the heliospheric current sheet. Submitted to *Geophysical Research Letters*. (LA-UR-22-24717)

*Fu, X., H. Li, Z. Gan, S. Du and J. Steinberg. Nature and Scalings of Density Fluctuations of Compressible Magnetohydrodynamic Turbulence with Applications to the Solar Wind. 2022. *The Astrophysical Journal*. **936** (2): 127. (LA-UR-22-32609 DOI: 10.3847/1538-4357/ac8802)

Gan, Z., H. Li, X. Fu and S. Du. On the Existence of Fast Modes in the Compressible Magnetohydrodynamic Turbulence. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-31374)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated Particle Acceleration in the Presence of Ambient Solar-Wind Turbulence. 2021. *Frontiers in Astronomy and Space Sciences*. **8**: 644354. (LA-UR-20-30411 DOI: 10.3389/fspas.2021.644354)

*Lazarian, A., G. L. Eyink, A. Jafari, G. Kowal, H. Li, S. Xu and E. T. Vishniac. 3D turbulent reconnection: Theory, tests, and astrophysical implications. 2020. *Physics of Plasmas*. **27** (1): 12305. (LA-UR-20-28591 DOI: 10.1063/1.5110603)

Lazarian, A., O. Khabarova, S. Xu and F. Guo. Violation of Flux Freezing, Turbulent Magnetic Reconnection and induced Particle Acceleration. Submitted to *Review of Modern Plasma Physics*. (LA-UR-21-27253)

*Liping, Y., L. Hui, G. Fan, L. Xiaocan, L. Shengtai, H. Jiansen, Z. Lei and F. Xueshang. Fast Magnetic Reconnection with Turbulence in High Lundquist Number Limit. 2020. *The Astrophysical Journal*. **901** (2): L22. (LA-UR-20-24765 DOI: 10.3847/2041-8213/abb76b)

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Yu, F., X. Kong, F. Guo, Y. Chen and J. Giacalone. Double-power-law feature in the energy spectra of energetic particles accelerated at coronal shocks. Submitted to *Astrophysical Journal*. (LA-UR-21-27255)

Presentation Slides

Conrad, E. K., J. T. Steinberg, R. M. Skoug, J. M. Broll, S. Du, H. Li, X. Fu and Z. Gan. Solar Wind Density Variability and Pressure Balance Near the Sun. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31868)

Conrad, E. K., J. T. Steinberg, R. M. Skoug, J. M. Broll, S. Du, H. Li, X. Fu and Z. Gan. Variability of Solar Wind Pressure Components & Pressure Balance Near the Sun. Presented at *Parker Solar Probe Ion Working Group Meeting (Virtual)*, Online, New Mexico, United States, 2022-08-16 - 2022-08-16. (LA-UR-22-28495)

Du, S. IC w22_compturb:Compressible Turbulence and Parametric Decay Instability in the Solar Wind. . (LA-UR-23-23036)

Du, S., H. Li, X. Fu, Z. Gan, F. Guo and X. Li. Magnetic Energy Conversion in Magnetically Dominated Systems and Implications for Particle Energization Processes. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31939)

Du, S., H. Li, X. Fu, Z. Gan and S. Li. Magnetic Energy Conversion in Magnetohydrodynamics: Curvature Relaxation and Perpendicular Expansion of Magnetic Fields. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30821)

Du, S., H. Li, X. Fu and Z. Gan. Anisotropic Energy Transfer and Conversion in Magnetized Compressible Turbulence. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30908)

Du, S., H. Li, X. Fu and Z. Gan. Density Fluctuations in Compressible Magnetohydrodynamic Turbulence: Connection between 3D Simulations and In-situ \xc2\xa0Solar Wind Observations. Presented at *Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2022-10-31 - 2022-11-04. (LA-UR-22-31534)

Du, S., H. Li, Z. Gan, X. Fu, E. K. Conrad, J. T. Steinberg and J. M. Broll. Anisotropic Compressible MHD Turbulence and Comparison with Parker Solar Probe Data. Presented at *Parker Two Conference*, Laurel, Maryland, United States, 2022-06-21 - 2022-06-24. (LA-UR-22-25638)

Li, H. 3D Turbulence with Global Reconnection. Presented at *19th Annual International Astrophysics Conference*, Santa

Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-28062)

Li, H. Turbulent Dynamo Modeling and Experiments using HED Plasmas. Presented at *AAPPS-DPP2020 On-line E-conference*, Pohang, Korea, South, 2020-10-26 - 2020-10-26. (LA-UR-20-28587)

Li, H. IC Project: Heating and Acceleration of Solar Wind by Parametric Decay Instability Mediated Turbulence. . (LA-UR-21-23434)

Li, H. Compressible MHD Turbulence and Implications for Solar Wind Turbulent Density Variations Measured by Parker Solar Probe. Presented at *Fundamentals of compressible turbulence: recent advances and open questions*, college station, Texas, United States, 2021-05-20 - 2021-05-21. (LA-UR-21-24830)

Li, H. Compressible MHD Turbulence and Implications for Solar Wind Turbulent Density Variations Measured by Parker Solar Probe. Presented at *The 2021 Midwest Magnetic Field Workshop*, Madison, Wisconsin, United States, 2021-06-14 - 2021-06-14. (LA-UR-21-25650)

Li, H. On the Existence of Finite Frequency Fast Modes in the Compressible MHD Turbulence. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-31375)

Li, H. Magnetic Energy Conversion in Magnetically Dominated Systems and Implications for Particle Energization Processes. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-31376)

Li, H. Spatio-Temporal Properties of Compressible MHD Turbulence and Implications. Presented at *Midwest Magnetic Fields*, Madison, Wisconsin, United States, 2022-05-23 - 2022-05-26. (LA-UR-22-24872)

Li, H. Heating and Acceleration of Solar Wind by Parametric Decay Instability Mediated Turbulence. . (LA-UR-22-25087)

Li, H. IC Project w20_solarwind: Heating and Acceleration of Solar Wind by Parametric Decay Instability Mediated Turbulence;. . (LA-UR-22-25088)

Li, H. Parametric Decay Instability of Alfven Waves in Low-Beta Astrophysical Plasmas. Presented at *64th Annual Meeting of the APS Division of Plasma Physics*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30905)

Li, H. Are There Waves in Magnetized Compressible Turbulence in Space and Astrophysical Plasmas. Presented at *64th Annual Meeting of the APS Division of Plasma Physics*, spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30906)

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Li, H. and X. Fu. Compressible Turbulence in the Solar Wind near the Sun. Presented at *19th AIAC Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-28061)

Posters

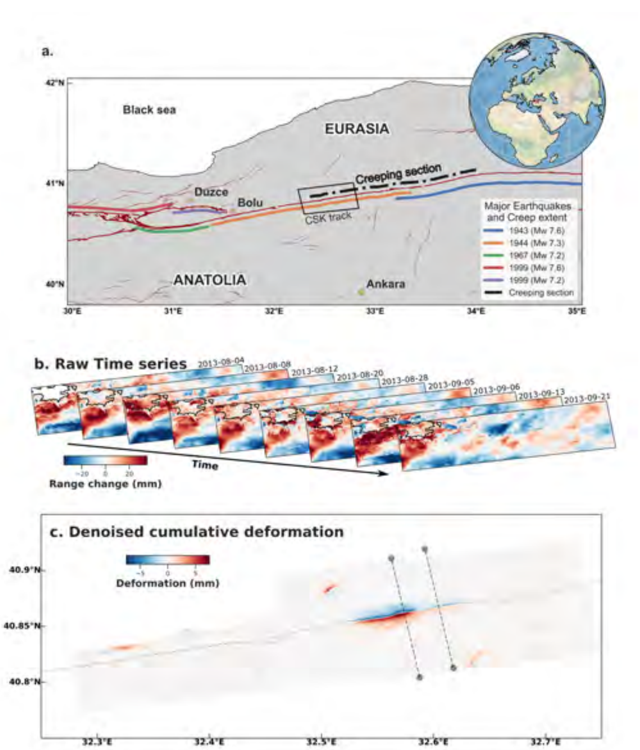
Conrad, E. K., J. T. Steinberg, R. M. Skoug, J. M. Broll, S. Du, H. Li, X. Fu and Z. Gan. Solar Wind Pressure Balance near the Sun: PSP Statistical Study. Presented at *Parker Two*, Laurel, Maryland, United States, 2022-06-21 - 2022-06-24. (LA-UR-22-25319)

Du, S., H. Li, X. Fu and Z. Gan. Spatial Filtering Analysis of Anisotropic Energy Transfer and Conversion in 3D Turbulence Simulations. Presented at *American Geophysical Union (AGU) Fall Meeting*, Chicago, Illinois, United States, 2022-12-12 - 2022-12-16. (LA-UR-22-32861)

**Peer-reviewed*

Deep Learning Interferometric Synthetic-Aperture Radar

Elena Reinisch
20200278ER



How do fault deformation events interact? What observable would allow to discriminate a harmless event from a precursor to a major earthquake? The answer to such fundamental questions requires to characterize the whole range of tectonic events - impossible given current observational gaps. The artificial intelligence the project team has developed unlocks the ability to monitor ground deformation with unprecedented precision, down to 1 millimeter as pictured here. Equipped with autonomous detection of deformation on faults, the team has the tool to close the gap in existing detection capabilities and form the foundations for a systematic exploration of the properties of active faults.

Project Description

Small ground deformations are associated with a variety of phenomena of critical importance: slow earthquakes, earthquakes precursors, aquifer levels variations, oil and gas extraction, water injection for geothermal applications, carbon dioxide sequestration, underground explosions, underground construction. Recent deployments of satellites for advanced radar imagery has enabled the unprecedented ability to monitor ground deformation globally. However, ground deformation maps acquired from radar interferometry suffers from very high levels of noise due to atmospheric disturbances and current state-of-the-art analysis relies on time consuming expert interpretation, preventing global detection of small deformations. We are developing a deep learning artificial intelligence specifically built to extract ground deformation signals of interest in interferometric synthetic aperture radar (InSAR) data. Our technology will unlock the ability to automatically monitor all deformations of interest globally, including small and slow deformations. The work will place the Laboratory at the forefront of underground deformation signature detection and induced earthquake mitigation. The approach we are developing also has application to ground based nuclear explosion monitoring, where even minute surface deformation signatures will become detectable. There will be applications to Fossil Energy, Carbon Sequestration and Geothermal problems, and to ongoing work funded by the Office of Science on deformation associated with faulting.

Technical Outcomes

This project aimed to advance the resolution capabilities of surface deformation detection in interferometric synthetic aperture radar time series and provide a method to detect such signals autonomously. The team accomplished both goals by developing a deep learning autoencoder to denoise time series deformation fields autonomously, detecting subtle (millimeter-scale) deformation signatures amidst atmospheric signal contamination. Successful applications to geophysical events demonstrate the method’s potential applicability to globally detect/monitor natural hazards and anthropogenic causes of deformation.

Publications

Journal Articles

Hulbert, C. L., B. P. G. Rouet-Leduc, P. A. Johnson and R. Jolivet. Automatic Tremor Location with Neural Network Interpretation. Submitted to *Geophysical Research Letters*. (LA-UR-20-22490)

Hulbert, C. L., B. P. G. Rouet-Leduc, P. A. Johnson and R. Jolivet. An exponential build-up in seismic energy suggests a months-long nucleation of slow slip in Cascadia. Submitted to *Nature Communications*. (LA-UR-19-29448)

Johnson, P. A. and B. P. G. Rouet-Leduc. Laboratory Earthquake Forecasting: A Machine Learning Competition. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-28829)

Licciardi, A., Q. Bletery, B. P. G. Rouet-Leduc, J. Ampuero and K. Juhel. Instantaneous Tracking of Earthquake Growth Using Prompt Elasto-Gravity Signals and Deep Learning. Submitted to *Nature*. (LA-UR-21-30873)

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Books/Chapters

G. Rouet-Leduc, B. P., C. X. Ren, C. L. Hulbert and P. A. Johnson. Machine learning and fault rupture: A review. (LA-UR-20-28827)

Reports

Angermeier, W., C. Barros, I. D. Dumitru, M. C. Holmes, J. R. Howard, S. R. Johnstun, G. B. King, J. T. Lindbloom, N. P. Lordi, A. Luu, S. E. Martinez, J. N. McBride, E. S. Nelluvelil, K. T. O'Dell, H. R. Pace, N. A. Poole, A. Ramkumar, S. M. Riedel, L. Singh, S. R. Venkat, D. A. Weatherred, J. Y. Wei, K. A. York, F. Yousuf, M. T. Andrews, D. M. Israel and J. A. Kulesza. Final Reports of the 2021 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-21-28941)

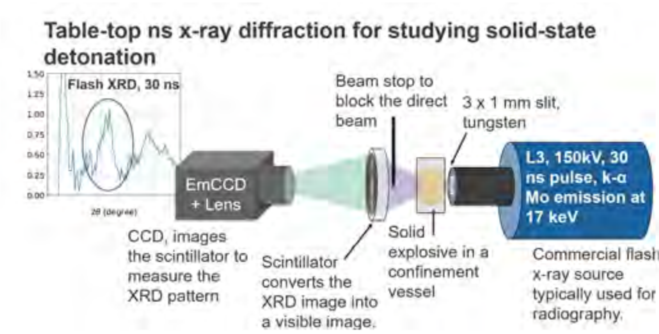
Presentation Slides

Ren, C. X., B. P. G. Rouet-Leduc, S. R. Venkat and K. T. O'Dell. Deep Learning for Satellite Imagery: Modelling Atmospheric Effects. . (LA-UR-21-27903)

**Peer-reviewed*

The Role of Defects in Solid State Detonation Kinetics

Pamela Bowlan
20200311ER



This project aims to measure the kinetics of solid-state detonation by time-resolving the loss of crystallinity during a detonation. To do this, the team will develop table-top nanosecond (ns) x-ray diffraction using flash x-ray sources which emit 30 ns pulses. Measuring the x-ray diffraction pattern at different times with respect to the detonation wave will allow the team to map out the kinetics. By the end of the project, the goal is to apply this to a triaminotrinitrobenzene (TATB) detonation.

Project Description

After decades of modeling and experiments, the physical mechanism by which a detonation occurs remains a mystery. Of particular interest to the Laboratory and national security are secondary solid explosives because of their relative insensitivity, but this lack of understanding seriously impedes our ability to predict their performance and safety. The reason for this uncertainty is not understanding how an impulse, such as an increase in temperature or pressure, leads to the fast chemistry that makes up a detonation wave. As a result, models have to infer the needed chemical rate equations from indirect measurements, which constrains the range of phenomena that can be predicted by a single model. The purpose of the work proposed here is to directly measure the kinetics of detonation in secondary explosives taking the nanosecond(ns)-time-scale loss of crystallinity to be the relevant progress variable. Our unique experimental approach can lead to a breakthrough study in explosives science that reveals the rate limiting step in detonation and an improved set of kinetics equations that can be implemented in reactive burn models, broadening the scope of phenomena that can be accurately predicted.

Technical Outcomes

This project focused on developing flash x-ray diffraction (XRD) for dynamic measurements on explosives using commercial nanosecond x-ray sources. The team successfully demonstrated flash XRD on metals and, for the first time, on organics. A surprising finding was that battery-powered, portable x-ray sources could be used for XRD. The team also worked towards a custom x-ray source for XRD and demonstrated that the method could be implemented in a vessel for future dynamic measurements.

Publications

Journal Articles

Bowlan, P. R., B. F. Henson, L. B. Smilowitz, N. A. Suvorova and D. M. (. Oschwald. Acceleration of thermal decomposition near the melting point in organic molecular crystals. Submitted to *Journal of Chemical Physics*. (LA-UR-20-22788)

Bowlan, P. R., N. A. Suvorova, D. K. Remelius, L. B. Smilowitz and B. F. Henson. Acceleration of thermal decomposition near the melting point in organic molecular crystals. Submitted to *Journal of Applied Physics*. (LA-UR-20-29950)

Bowlan, P. R., N. A. Suvorova, D. K. Remelius, L. B. Smilowitz and B. F. Henson. Tracking thermal decomposition chemistry in secondary solid explosives with x-ray diffraction. Submitted to *Journal of Physical Chemistry A*. (LA-UR-21-25685)

Bowlan, P. R., N. A. Suvorova, D. K. Remelius, L. B. Smilowitz and B. Henson. Tracking thermal decomposition chemistry in organic crystalline solids with x-ray diffraction. Submitted to *Journal of Physical Chemistry A*. (LA-UR-21-31193)

Presentation Slides

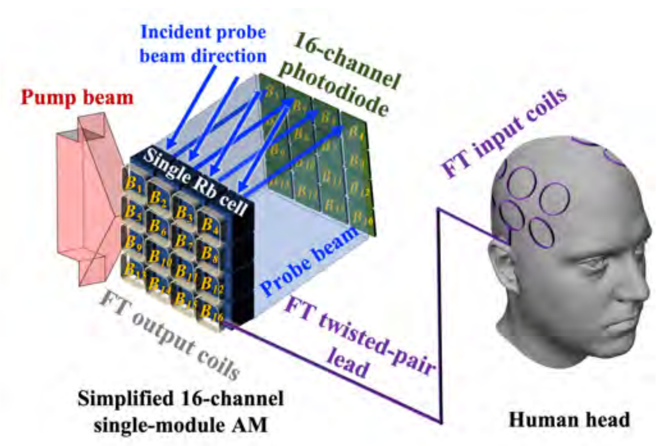
Bowlan, P. R. High explosives detection through containers using portable x-ray diffraction. Presented at *PROACTIVE NA-22 Venture workshop*, Oakridge, Tennessee, United States, 2022-11-15 - 2022-11-18. (LA-CP-22-20879)

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius and N. A. Suvorova. Time resolving the loss of crystallinity during detonation in a solid explosive. Presented at *APS March Meeting*, virtual meeting, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22332)

**Peer-reviewed*

Parallel Magnetic Resonance Imaging with a Multichannel Radio-Frequency Atomic Magnetometer

Young Jin Kim
20200393ER



Current multichannel ultra-low field magnetic resonance imaging (ULF MRI) systems present multiple technical challenges due to cryogenic operation. A more practical multichannel ULF MRI system based on an innovative multichannel single-module atomic magnetometer (AM) coupled to multiple flux transformers (FTs) will be demonstrated to advance the current technology. The new approach by removing the need for cryogens and realizing a large number of channels in a single module reduces cost, improves resolution, and leads to portable, parallel ULF MRI.

Project Description

The goals of this project are (1) to construct a new ultra-low field (ULF) magnetic resonance imaging (MRI) system based on a novel technique of a multichannel single-cell radio-frequency (RF) atomic magnetometer (AM) with multiple flux transformers (FTs) and demonstrate high sensitivities in each sensing channel in an unshielded environment; (2) to perform feasibility proof by initial parallel MRI experiments using a water phantom; (3) to demonstrate its application in accelerated MRI measurements of human subject such as a human brain, hand, and spine, which will be an exciting event for the biomedical community. This project will lead to cost-effectiveness and image acceleration, which will be an important revolution and a major breakthrough in biomagnetic diagnostics leading to new medical applications. In addition, it will put Los Alamos in the leading position in novel imaging applications, including in medical imaging and nuclear quadrupole resonance (NQR) imaging for explosive detection, and will be a unique capability in multichannel RF AM.

Technical Outcomes

The team has optimally designed and constructed prototype 16-channel and single-channel systems. Using the single-channel system, the team demonstrated magnetic resonance imaging of the water phantom with high resolution of 1 mm in the total acquisition time of 6.3 min in a single scan without averaging. Since the 1 mm resolution is typical in anatomical medical imaging, this method can be an alternative low-cost, rapid, portable anatomical medical imaging of the human body or animals.

Publications

Journal Articles

*Kim, Y. J. and I. M. Savukov. Parallel high-frequency magnetic sensing with an array of flux transformers and multi-channel optically pumped magnetometer for hand MRI application. 2020. *Journal of Applied Physics*. **128** (15): 154503. (LA-UR-20-24994 DOI: 10.1063/5.0021284)

Savukov, I., Y. J. Kim and S. Newman. High-resolution ultra-low field magnetic resonance imaging with a high-sensitivity sensing coil. 2022. *Journal of Applied Physics*. **132** (17): 174503. (LA-UR-22-29121 DOI: 10.1063/5.0123692)

*Savukov, I. and Y. J. Kim. Investigation of magnetic noise from conductive shields in the 10-300\xe2\x80\x89kHz frequency range. 2020. *Journal of Applied Physics*. **128** (23): 234501. (LA-UR-20-27307 DOI: 10.1063/5.0029998)

Presentation Slides

Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)

Kim, Y. J., I. M. Savukov and S. G. Newman. Magnetic Resonance Imaging (MRI) with a Multichannel Optically Pumped Magnetometer. Presented at *APS March Meeting 2022*, CHICAGO, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22078)

Kim, Y. J. and I. M. Savukov. Development of a multichannel atomic magnetometer for parallel magnetic resonance imaging. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21897)

Savukov, I. M. and Y. J. Kim. Broadband Ultra-sensitive Adiabatic Magnetometer. Presented at *SAS 2012*, Virtual, Sweden, 2021-08-23 - 2021-08-25. (LA-UR-21-27516)

Savukov, I. M. and Y. J. Kim. Multi-channel radio-frequency optically pumped magnetometers and their applications in MRI. Presented at *Virtual WOMP meeting*, Berlin, Germany, 2021-10-04 - 2021-10-05. (LA-UR-21-29802)

Posters

Kim, Y. J., I. M. Savukov and S. G. Newman. Parallel Ultra-low Field Magnetic Resonance Imaging with a Multichannel Optically Pumped Magnetometer. Presented at *Experimental Nuclear Magnetic Resonance Conference 2022*, Orlando, Florida, United States, 2022-04-24 - 2022-04-29. (LA-UR-22-23641)

Kim, Y. J., I. M. Savukov and S. G. Newman. Parallel Ultra-low Field Magnetic Resonance Imaging with Atomic Magnetometers. Presented at *International Council on Magnetic Resonance in Biological Systems 2022 Conference*, Boston, Massachusetts, United States, 2022-08-21 - 2022-08-25. (LA-UR-22-28684)

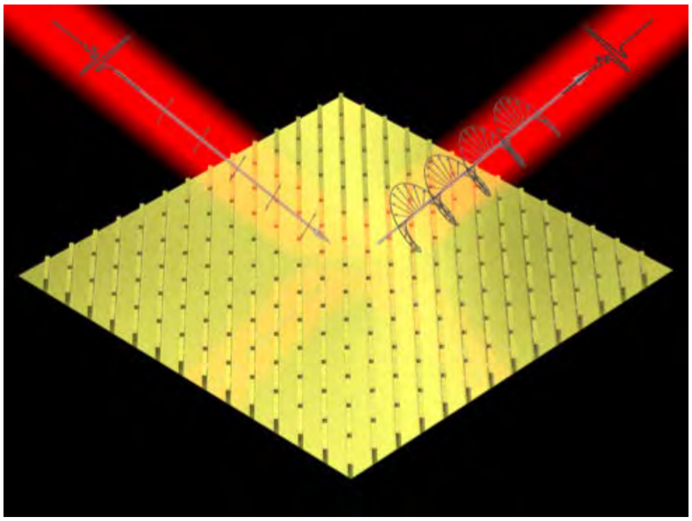
Savukov, I. M. and Y. J. Kim. Development of multi-channel parallel atomic magnetometer MRI. Presented at *Practical Applications of NMR in Industry Conference (PANIC 2020) --Virtual meeting*, Los Alamos, New Mexico, United States, 2020-10-19 - 2020-10-22. (LA-UR-20-27922)

Savukov, I. M. and Y. J. Kim. Toward Multi-channel Magnetic Resonance Imaging with Radio-frequency Atomic Magnetometers. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Atomic, Molecular and Optical Physics (DAMOP)*, Orlando, Florida, United States, 2022-05-30 - 2022-06-03. (LA-UR-22-24818)

**Peer-reviewed*

Broadband Terahertz Circular Dichroism Spectroscopy

Houtong Chen
20200419ER



A micro-fabricated reflective metasurface structure that allows the conversion of linearly polarized incident terahertz waves to circularly polarized reflection over one octave bandwidth. Scaling the structural dimensions allows the device to operate at different frequency bands, thereby covering the entire terahertz bandwidth of interest. Rotating the incident linear polarization by 90 degree results in the conversion of circular polarization with opposite handedness, making the device the most critical component in the development of a broadband terahertz circular dichroism spectrometer for the measuring the optical response of a wide range of chiral biomolecules.

Project Description

Although the richness of terahertz (THz, or far-infrared) spectral fingerprints in large biomolecules makes THz circular dichroism (THz-CD) spectroscopy an extremely important tool to detect functionally relevant dynamic modes, currently there is no existence of any THz-CD system for practical use due to the lack of high-performance THz circular polarization modulators. We tackle this long-standing challenge by taking advantage of our recent patent-pending metasurface technology, which allows us to develop, for the first time in the world, a broadband THz-CD spectrometer and measure the rich signature of global dynamic modes and conformation changes within large chiral biomolecules. The success of the proposed work, including the instrumentation itself and the corresponding scientific discoveries utilizing this instrument, will pave an avenue to solve problems in biochemistry, drug discovery, and food research laboratories and industries. Upon the completion of this project, the anticipated deliverables include: a) A set of high-performance, broadband THz metasurface circular polarization modulators cover the entire THz band; b) A THz-CD spectrometer for measurements of chiral biomolecules and biomaterials; c) A set of THz CD spectroscopy data first ever for a variety of biomolecules related to molecular structures and functions.

Technical Outcomes

A new theoretical mechanism was identified for broadband linear-to-circular polarization conversion based through deliberately designing unique phase dispersion in reflective metal-dielectric-metal metasurface cavities exhibiting birefringent Fabry-Pérot-like resonances. Both numerical simulations and experimental works were carried out and validated this novel concept at terahertz frequencies, showing linear-to-circular polarization conversion with near-unity conversion efficiencies and over one octave bandwidth, scalable to operate at any other arbitrary frequency range, either at normal incidence or at oblique incident angles.

Publications

Journal Articles

*Chang, C., Z. Zhao, D. Li, A. J. Taylor, S. Fan and H. Chen. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. 2019. *Physical Review Letters*. **123** (23): 237401. (LA-UR-18-31108 DOI: 10.1103/PhysRevLett.123.237401)

Chen, H., S. R. M. Silva, C. Corbella, A. D. Tang, P. Nath and A. K. Azad. Microwave Metasurface-Based Alvarez Lens. Submitted to *Applied Physics Letters*. (LA-UR-20-30096)

Chen, H., W. Xu, W. Fang, T. Shi, X. Ming, Y. Wang, L. Xie, L. Peng and Y. Ying. Wafer-Scale Carbon Nanofilms for Plasmonic Terahertz Devices and Sensors. Submitted to *Nature Electronics*. (LA-UR-22-24303)

Chen, H., Y. Zhang, T. Wang, J. Guo and X. Wang. High efficiency spatial terahertz modulator. Submitted to *Journal of Applied Physics*. (LA-UR-21-30748)

Chen, H., Z. Zhao, D. Li, A. J. Taylor, S. Fan and C. Chang. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. Submitted to *Physical Review Letters*. (LA-UR-19-29771)

Pettine, J. A., P. Padmanabhan, N. S. Sirica, R. P. Prasankumar, A. J. Taylor and H. Chen. Ultrafast Terahertz Emission from Emerging Symmetry-Broken Materials. Submitted to *Light: Science & Applications*. (LA-UR-23-20217)

Zhu, L., Z. Sheng, H. Schneider, H. Chen and M. Tani. Ultrafast phenomena and terahertz waves: introduction. 2022. *Journal of the Optical Society of America B*. **39** (3). (LA-UR-22-31499 DOI: 10.1364/JOSAB.457128)

Presentation Slides

Chen, H. Metasurfaces accomplish ultra-broadband optical polarization conversions. Presented at *CLEO Pacific Rim*, Sydney, Australia, 2020-08-03 - 2020-08-03. (LA-UR-20-25943)

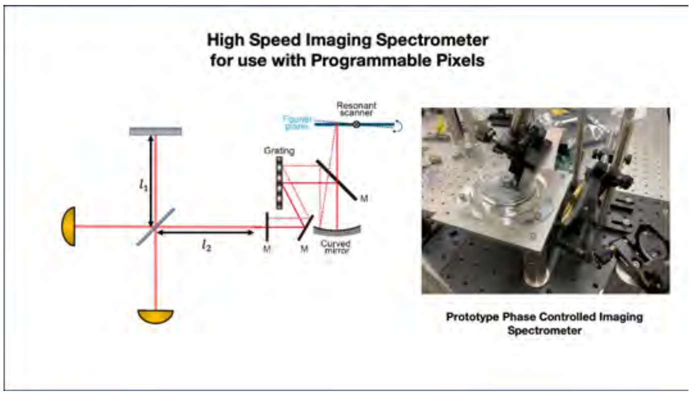
Chen, H. Metasurface Broadband Polarization Converters Towards Terahertz Circular Dichroism Spectroscopy. Presented at *IRMMW-THz 2020*, Buffalo, New York, United States, 2020-11-08 - 2020-11-13. (LA-UR-20-30097)

Chen, H. Ultrafast Nanoscale Photocurrent Control and Terahertz Emission with Symmetry-Broken Optoelectronic Metamaterial. Presented at *OTST 2022*, Budapest, Hungary, 2022-06-19 - 2022-06-24. (LA-UR-22-25837)

**Peer-reviewed*

Gleaming the Cube: Advanced Focal Planes for Optimal Acquisition of Spectral Images

John Bowlan
20210306ER



Hyperspectral imaging is an important technique for remote sensing and microscopy. Los Alamos researchers are developing new instruments which combine novel optics with digital pixels to optimize the acquisition of hyperspectral images. These optimizations will improve acquisition speed, spectral resolution, and signal-to-noise ratio. [Image credit: Los Alamos National Laboratory]

Project Description

A hyperspectral image (HSI or data cube) is an image where hundreds of spectral channels are acquired for every pixel. It is a powerful remote sensing technique that can passively identify the spectral signatures of materials from up to 100's of km away. Current state-of-the art HSI systems make inefficient use of available light because the same acquisition settings must be used for all areas of an image. We will develop a prototype image sensor using a novel focal plane array (FPA) design that is optimized for the acquisition of hyperspectral images. We expect significant improvements over the current state-of-the-art in frame-rate and signal-to-noise (SNR), while avoiding the traditional engineering trade-offs against spectral resolution. These gains are achieved by allowing each pixel to adapt to the dynamic characteristics the scene. Our proposed design exploits recent advances in infrared focal plane arrays, and aims to enable the application of passive spectral imaging to scenarios where it is not currently practical, such as handheld operation and acquisition of moving objects. The improved sensitivity will also enable the detection of entirely new classes of spectral signatures that are beyond the capabilities of today's technology.

Technical Outcomes

The objective of this project was to develop optical and camera readout technologies that have the potential to dramatically improve the performance of hyperspectral sensors. This project successfully built a candidate imaging interferometer and thoroughly analyzed its performance and limitations. These experimental and design results represents significant technical progress toward the goal. This approach has the potential to lead to dramatic improvements in the performance (temporal resolution and signal-to-noise) of hyperspectral imaging systems.

Publications

Conference Papers

Thurmond, K. D. and J. M. Bowlan. Analysis of Phase-Controlled Fourier Transform Spectroscopy for Remote Sensing Applications. Presented at *optica optical sensor and sensing congress*. (Vancouver, Canada, 2022-07-11 - 2022-07-15). (LA-UR-22-22468)

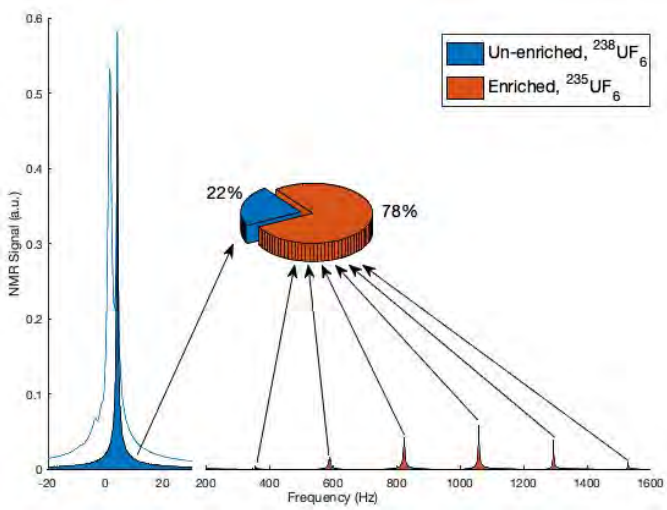
Presentation Slides

Thurmond, K. D. and J. M. Bowlan. Analysis of Phase-Controlled Fourier Transform Spectroscopy for Remote Sensing Applications. Presented at *optica optical sensor and sensing congress*, Vancouver, Canada, 2022-07-11 - 2022-07-15. (LA-UR-22-26216)

**Peer-reviewed*

Uranium Hexafluoride Enrichment Verification Using Ultra-Low Field Nuclear Magnetic Resonance

Per Magnelind
20210770ER



Verifying uranium enrichment is critical for nuclear safeguards. This project will develop a new direct method to precisely determine uranium enrichment in the field and improve nuclear safeguards. The method is based on comparing nuclear magnetic resonance (NMR) signals from un-enriched (U-238; blue area) and enriched (U-235; red areas) uranium hexafluoride, UF6, detected in very weak magnetic field. To enhance NMR signals, the target sample pre-polarized in a stronger magnetic field is moved into a shielded environment for detection.

Project Description

As new, large capacity, Gas Enrichment Centrifuge Plants (GECPs) are brought online, the inspection effort by the International Atomic Energy Agency that safeguards these facilities is an increasing burden. Verifying uranium enrichment is a key objective for GECP safeguards. Existing technologies have a variety of strengths and weaknesses. Measurements are technically very challenging and prone to spoofing in high background radiation or highly dynamic production environments with conventional methods. However, Nuclear Magnetic Resonance (NMR) has the potential to improve the performance of such measurements, as it is inherently not sensitive to radiation and allows accurate measurement inside non-magnetic metallic packaging such as pipes with enriched Uranium hexafluoride (UF6) gas. NMR provides a unique multi-peak signature from enriched UF6 (uranium-235), as it is the only long half-life Uranium-isotope with a non-zero spin property. However, conventional NMR is not fieldable and cannot detect usable signals through pipes or containers. The zero to ultra-low field (ZULF) regime, 0–500 Nanoteslas (nT), has the potential for a portable/fieldable NMR technique to measure uranium enrichment. The method is non-invasive, can measure inside non-magnetic metallic packaging, and does not rely on ionizing radiation. An improved non-destructive enrichment verification technology would benefit onsite inspections of nuclear facilities worldwide.

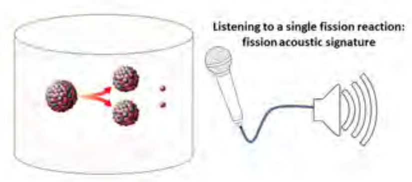
Technical Outcomes

The project successfully leveraged existing hardware and new acquisitions to assemble a system targeted at performing nuclear magnetic resonance in magnetic fields strengths at a fraction of Earth's magnetic field. The team demonstrated that the system can detect both the peak at a couple of hertz and at least the first peak at ~1 kilohertz for lithium hexafluorophosphate(LiPF6), which is also a hexafluoride with a spectrum with some similarities to our target material UF6 (uranium-235).

Fission-Acoustic Signature Discovery

Rollin Lakis

20210853ER



The objective of this work is to lay the foundation for the first experiments to "listen" for the sound of an individual fission event. When successful, this new signature will open many possibilities for the characterization of fissile materials in condensed matter, to study the evolution of defects in condensed matter and to potentially image fission events under extreme conditions.

Project Description

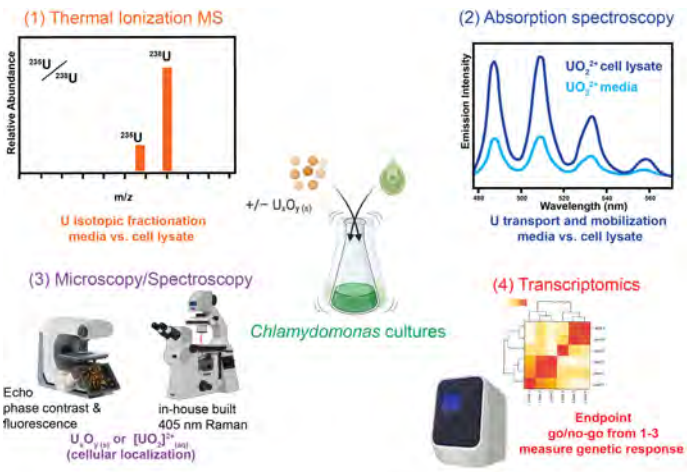
The objective of this work is to lay the foundation for the first experiments to "listen" for the sound of an individual fission event. When successful, this new signature will open many possibilities for the characterization of fissile materials in condensed matter, to study the evolution of defects in condensed matter and to potentially image fission events under extreme conditions. The fission-acoustic measurement can, in addition, open opportunities detect and characterize high consequence objects, and to monitor actinide processes.

Technical Outcomes

An experiment was performed to detect the acoustic response of spontaneous fission in a small single crystal of uranium dioxide. There were observable features in the vibrometry data that might represent an acoustic signature for fission. However, the team was not willing to declare the first detection of acoustic fission signatures under these circumstances. Molecular dynamics modeling was also performed to estimate the total acoustic energy possible from a fission event in uranium dioxide.

Rapid Bioremediation and Simultaneous Enrichment of Uranium by Common Green Algae

Laura Lilley
20210869ER



Some species of green algae can uptake and isotopically fractionate uranium (U-235/238) with implications across bioremediation and national security. Through a suite of four experiments, the project team will elucidate the primary mechanism of this process in live green algae. This will be accomplished through; 1) thermal ionization mass spectroscopy (TIMS) informing isotopic fractionation and localization of uranium, 2) optical spectroscopy determining uranium speciation and relative bulk concentrations, 3) optical and fluorescent microscopy/spectroscopy informing cellular localization, and 4) RNA will be extracted and transcriptomic experiments will investigate the genetic differences between uranium-exposed and control experiments.

Project Description

Research in green algae is a cornerstone of Department of Energy (DOE) research initiatives; isotopic fractionation is a cornerstone in the National Nuclear Security Administration (NNSA) mission space. Based on the observation that green algae are capable of uranium uptake and isotopic fractionation, we are investigating the mechanisms through which this process is governed. This fundamental understanding will enable us to 1) manipulate the uptake (bioremediation) and fractionation (energy) in cultures of green algae, 2) evaluate and anticipate potential clandestine threats (forensics), and 3) investigate a new research avenue for biologically-mediated isotopic separations (separation science).

Technical Outcomes

Here, the team sought to investigate the capability of green algae to fractionate uranium-235 from 238. This project has advanced the field of bioremediation significantly. We demonstrated that a naïve strain of green algae could be acclimatized to very large quantities of uranium – 800 microgram/milliliter while being able to uptake approximately one-third of the total uranium in solution. This presents a unique opportunity for bioremediation efforts.

Understanding Optical Signatures from Natural and Artificial Aurora

Rebecca Sandoval
20200555ECR

LDRD researcher Rebecca Holmes Sandoval with LANL's NCam single-photon camera in Fairbanks, Alaska, with the aurora in the background. Data on the natural aurora will help develop techniques for assessing performance of space accelerators from the ground, a valuable diagnostic tool for future science and security missions. These observations also captured the fastest video of the aurora ever recorded, which is expected to lead to important scientific discoveries about where the aurora originates

Project Description

Research using particle accelerators in space is critical to understanding how space weather affects the Earth, including negative effects on satellites and power grids. Space accelerators also have security applications, including reducing the impact of space radiation from a high-altitude nuclear explosion. Measuring accelerator performance in space, where laboratory instruments are not available, is a major challenge for developing the technology that enables these important missions. This project will develop a better way to measure accelerator performance by using an ultra-sensitive camera on the ground to capture the light produced when the beam from a space accelerator hits the atmosphere. First, we will develop measurement techniques by observing the natural aurora (Northern Lights), which produces a similar type of light. These tests will also capture the fastest video of the aurora ever recorded, which is expected to lead to important scientific discoveries about where the aurora originates. After developing experimental techniques by observing the aurora, we will actually measure the light from a space accelerator for the first time. By showing that we can assess how an accelerator performs from the ground, we will develop a valuable diagnostic tool for future science and security missions.

Publications

Presentation Slides

Sandoval, R. H. Space Research at Los Alamos National Laboratory. . (LA-UR-21-21850)

Other

Sandoval, R. H. and E. K. Emberton. Aurora photos for LDRD 20200555ECR. Audio/Visual. (LA-UR-21-24195)

**Peer-reviewed*

A High-Throughput (RapidPhage) Platform for the Discovery of Lytic Bacteriophages Against Multi-drug Resistance Pathogens

Anand Kumar
20210612ECR

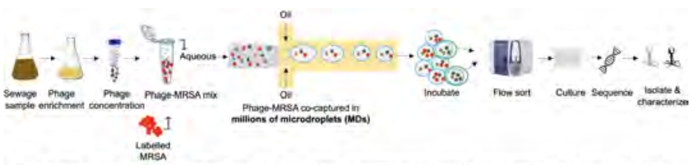


Figure 1. Overview of RapidPhage screening platform with an example of the rapid discovery and isolation of MRSA-lytic novel phages from the sewage sample

The use of bacteriophage to treat multidrug resistant infections has shown promise but, rapid discovery and isolation of such novel and effective bacteriophages remain significant challenges. Here the team aims to develop a RapidPhage platform and demonstrate its utility by discovering methicillin-resistant Staphylococcus aureus (MRSA) bacteriophages. The successful demonstration of this platform will greatly improve the discovery and isolation of effective bacteriophages against any bacterial pathogen (including multi-drug resistant) of plant, animal and human hosts.

Project Description

The universal decline in the effectiveness of antibiotics, combined with the dearth of newer antibiotics and the emergence of hard-to-treat bacterial pathogens, have driven the need to revisit alternatives to antibiotics. The use of bacteriophage therapy has shown assurance in addressing hard-to-treat bacterial pathogen infections but unfortunately, rapid discovery and isolation of novel phages remain significant challenges. The current gold standard technique to discover and isolate phages against specific pathogens relies on a classical plaque formation assay, which is low throughput, inefficient, and cumbersome. To overcome these limitations and advance the rapid discovery of therapeutic phages, we propose to develop a novel, widely applicable, high-throughput platform (named RapidPhage) to rapidly discover, isolate and characterize lytic phages against pathogens. As a proof of concept, we will apply the RapidPhage platform to discover methicillin-resistant Staphylococcus aureus (MRSA)-lytic phages. The outcome from this study will provide a novel, widely-applicable platform, which will substantially improve the discovery and isolation of lytic phages that are effective against the target pathogen of interest.

Publications

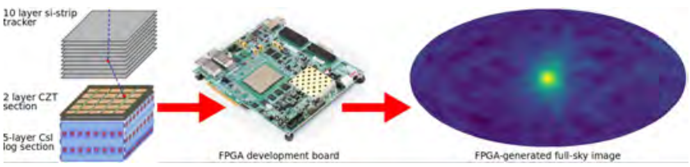
Posters

Abernathy, G. A., A. Kumar, A. M. C. Waller and A. E. K. Dichosa. RapidPhage: a microfluidic based phage isolation platform to combat antibiotic resistant pathogens. Presented at *New Mexico Research Symposium*, Albuquerque, New Mexico, United States, 2022-11-05 - 2022-11-05. (LA-UR-22-31703)

**Peer-reviewed*

Locating Nature's Most Extreme Explosions in Real-Time

Lucas Parker
20210675ECR



This project develops a new technology: a completely FPGA-based pipeline that analyzes data from Compton telescopes to discover and localize gamma-ray bursts in the maximal extractable value (MeV). Left is a schematic of the ComPair gamma-ray telescope, which is the targeted demonstration instrument, set to fly from a balloon. Data from ComPair will be analyzed during the balloon flight by a low-power FPGA board, represented in the center. The Compton analysis will trigger when a burst is detected, generating maps similar to what shown on the right, ultimately localizing gamma-ray bursts within milliseconds.

Project Description

CubeSats have been a disruptive force in the space industry, substantially reducing the cost and development time required to reach orbit, making it possible to rapidly deploy new space-based instruments. CubeSats and small satellites in general are now used for "agile space" national security missions. As an example, for monitoring applications a constellation of small satellites has clear advantages over that of a single large satellite. An obvious disadvantage of small satellites is their limited power budget, which in turn caps the computing capability of an instrument. How smart can a small satellite-borne instrument be if it only has a few watts of power allocated for computing? This project will pioneer the use of field programmable gate arrays (FPGAs) to perform the complex data analysis required for gamma-ray telescopes, achieving the high performance necessary for our analysis to be performed in real-time. FPGAs are a low-power computing resource, well suited for use on small satellites. This project targets an astrophysical application, but the employed techniques, including the use of artificial intelligence, can be applied to perform sophisticated edge computing on-board small satellites used for national security.

Publications

Journal Articles

Caputo, R., C. L. Fryer and L. P. Parker. The All-sky Medium Energy Gamma-ray Observatory eXplorer (AMEGO-X) Mission Concept. Submitted to *Journal of Astronomical Instrumentation*. (LA-UR-22-24203)

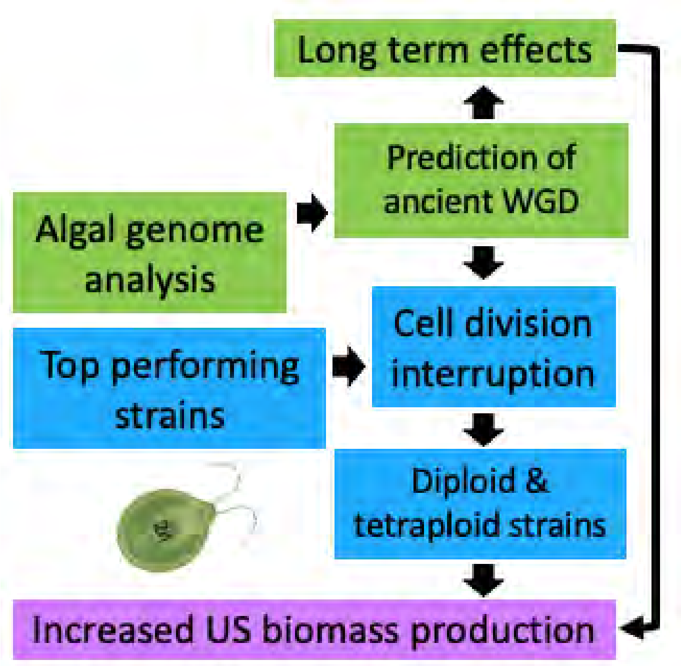
Parker, L. P., R. Datta, M. K. Brewer, J. Denes Couto, J. Eimer, Y. Li, Z. Xu, J. Appel, C. Bennett, R. Bustos, D. Chuss, S. Dahal, F. R. J. Espinoza Inostroza, K. Harrington, J. Iuliano, T. Marriage, C. N\xc3\xba\xc3\xb1ez, I. Padilla, R. Reeves, K. Rostem, D. A. Nunes Valle, D. Watts, J. Weiland and E. Wollack. Cosmology Large Angular Scale Surveyor (CLASS): 90 GHz Telescope Pointing, Beam Profile, Window Function, and Polarization Performance. Submitted to *Astrophysical Journal*. (LA-UR-22-31380)

Parker, L. P., S. Dahal, J. W. Appel, R. Datta, M. K. Brewer, A. Ali, C. L. Bennett, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. D. Couto, K. L. Denis, R. Dunner, J. Eimer, F. Espinoza, T. Essinger-Hileman, J. E. Colec, K. Harrington, K. Helson, J. Iuliano, J. Karakla, Y. Li, T. A. Marriage, J. McMahon, N. J. Miller, S. Novack, C. Nunez, K. Osumi, I. L. Padilla, G. Palma, M. A. Petroff, R. Reeves, G. Rhoades, K. Rostrem, D. A. N. Valle, D. J. Watts, J. L. Weiland, E. J. Wollack and Z. Xu. Four-year Cosmology Large Angular Scale Surveyor (CLASS) Observations: On-sky Performance at 40, 90, 150, and 220 GHz Frequency Bands. Submitted to *Astrophysical Journal*. (LA-UR-21-25008)

**Peer-reviewed*

Increasing the Nation's Energy Resilience through Whole Genome Duplicated Algae

Erik Hanschen
20220554ECR



How computational (green) and empirical (blue) analyses will combine to predict ancient whole genome duplication (WGD) in algae to selection and prediction of top performing biofuel-relevant production algae to create strains with double (diploid) and quadruple (tetraploid) the amount of natural, non-transgenic DNA within a cell. These algae will grow faster and be more robust to changes in an environment, resulting in increased US biomass production.

Project Description

Renewable energies based on biofuels require fast and reliable growth of production crops. However, despite their importance to biofuel production in the United States, little research into the use of whole genome duplication in algae has occurred. Whole genome duplication doubles the amount of natural, non-transgenic Deoxyribonucleic acid (DNA) inside a cell, which allows cells to grow and divide much more quickly. By artificially creating cells with double and quadruple the amount of natural, non-transgenic DNA inside an algae cell, we will be able to increase the growth rate of biofuel production algal crops, increasing the production of renewable biofuel energy.

Publications

Journal Articles

Biondi, T. C., C. P. Singer Kruse, S. I. Koehler, T. Kwon, W. L. K. M. Eng, Y. A. Kunde, C. D. Gleasner, K. T. You Mak, J. E. W. Polle, B. Hovde, E. R. Hanschen and S. R. Starkenburg. Assembly and analysis of the 100% complete, gapless, phased diploid genome of Scenedesmus obliquus UTEX 3031. Submitted to *Nucleic Acids Research*. (LA-UR-22-31391)

Jebali, A., M. R. Sanchez, E. R. Hanschen, S. R. Starkenburg and A. A. Corcoran. Trait drift in microalgae and applications for strain improvement. Submitted to *Biotechnology Advances*. (LA-UR-23-23300)

Jim\xc3\xa9nez-Mar\xc3\xadn, B., J. B. Rakijas, A. Tyagi, A. Pandey, E. R. Hanschen, J. Anderson, M. G. Heffel, T. G. Platt and B. J. S. C. Olson. Gene loss during a transition to multicellularity. Submitted to *Scientific Reports*. (LA-UR-23-23299)

Presentation Slides

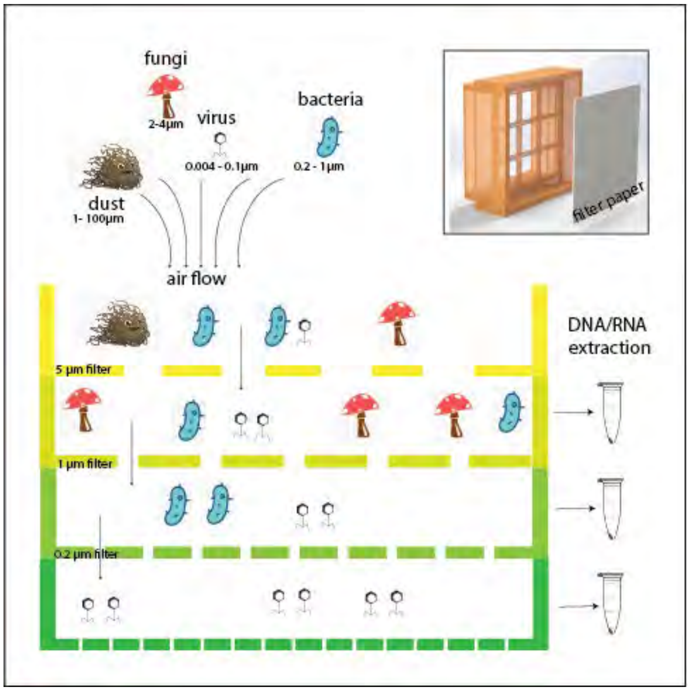
Hanschen, E. R. Enrichment of threat agent DNA from samples for identification and tracking. . (LA-UR-23-22877)

You Mak, K. T. From Burke's to Biologist. . (LA-UR-23-23073)

**Peer-reviewed*

A Next Generation Biosurveillance System for Detecting and Monitoring Threats

Migun Shakya
20220585ECR



Direct sampling and sequencing of complex mixture samples such as air and wastewater increases noise and obfuscates signals important for pathogen detection. To address this issue, the project team will use tiered sampler that separates mixtures based on their sizes before sequencing.

Project Description

An effective biosurveillance methods is key in detecting novel pathogens and mitigating damages from their outbreaks. The current pandemic has shown that wastewater and air surveillance using Next Generation Sequencing methods are capable of detecting circulating variants of Severe Acute Respiratory Syndrome-Coronavavirus 2 (SARS-CoV-2) even before actual outbreaks. One of the reasons this approach has been so successful during the current pandemic, but less so for other surveillance efforts, is because these methods have been tailored to specifically target SARS-CoV-2. A broad biosurveillance method that can detect wide array of pathogens as well as describe genetic traits related to their pathogenesis (E.g. presence of specific genes) are lacking. Some of the hurdles for delivering such biosurveillance system is separating important genetic signals from complex samples, all while making it deployable and cost effective. As technologies required for this kind of system, such as sequencing, computation, manufacturing, and bioinformatics have made significant improvements in recent years, we plan to work towards a next generation biosurveillance system by combining advancements from different fields.

Publications

Posters

Ruth, N. D., B. J. Youtsey, P. S. G. Chain, A. J. Hatch and M. Shakya. Optimization and Development of Technologies for Environmental Biosurveillance. Presented at *Chemical and Biological Defense Science and Technology (CBD S&T) Conference*, san fransisco, California, United States, 2022-12-06 - 2022-12-06. (LA-UR-22-31599)

Ruth, N. D., B. J. Youtsey and M. Shakya. What's lurking in your sewer? Assessing microbial diversity using public data. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27796)

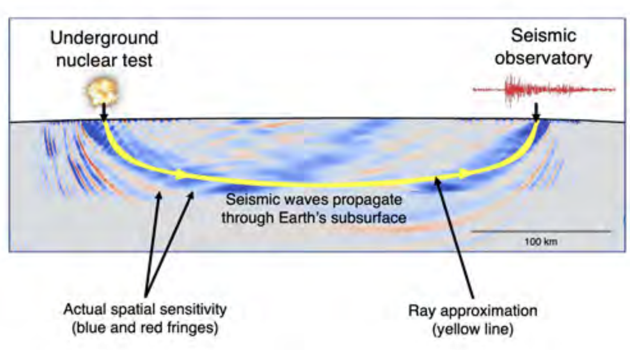
Ruth, N. D., B. J. Youtsey and M. Shakya. What's lurking in your sewer? Assessing microbial diversity using public data. Presented at *Los Alamos National Laboratory (LANL) Student Symposium*, Los Alamos, New Mexico, United States, 2022-08-01 - 2022-08-03. (LA-UR-22-27798)

**Peer-reviewed*

High-Frequency Explosion Monitoring Based on Waveform Discriminants

Ryan Modrak

20220592ECR



National security agencies use seismic stations to detect underground nuclear explosions. Current explosion monitoring, however, relies on mathematical approximations that become less reliable for small explosions, such as North Korea's 2006 declared nuclear test. For high-frequency crustal seismic waves generated by such explosions, ray approximations (yellow line) diverge significantly from actual propagation paths (red and blue fringes). The proposed work aims to improve low-yield explosion monitoring capabilities by developing new methods based on accurate wave-path modeling.

Project Description

To detect underground nuclear explosions, national security agencies rely on seismograms similar to those used by earthquake seismologists. Identifying explosions using these data becomes more challenging for smaller seismic events or for events observed at fewer stations. The proposed work aims to improve monitoring of small explosions by more accurately modeling seismic waves. Rather than individual seismic phases our approach involves entire seismic waveforms, making it possible to incorporate accurate waveform modeling and to avoid inaccurate ray approximations. Additionally, we seek to address operational challenges faced by national security agencies. By avoiding the need to manually identify individual P waves, our approach frees analyst time and makes it possible to more thoroughly screen for underground explosions.

Publications

Journal Articles

Nelson, P. L., R. T. Modrak, W. S. Phillips and M. L. Begnaud. Finite-Frequency Kernels for Pg Wavetrains. Submitted to *BSSA*. (LA-UR-22-27777)

Thurin, J., C. Tape and R. T. Modrak. Multi-Event Explosive Seismic Source for the 2022 Mw\xc2\xa06.3 Hunga Tonga Submarine Volcanic Eruption. 2022. *The Seismic Record*. **2** (4): 217-226. (LA-UR-22-29916 DOI: 10.1785/0320220027)

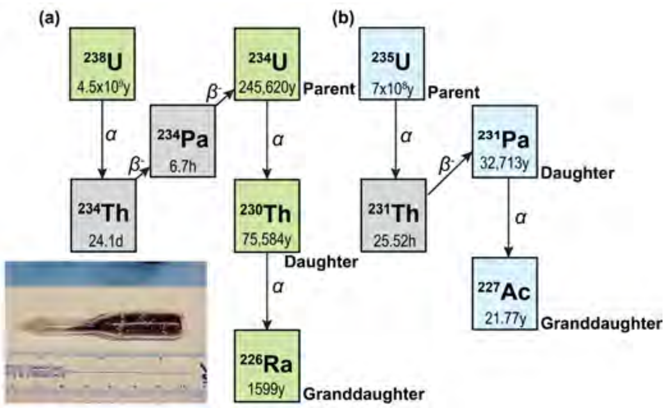
Reports

Modrak, R. T. Robust explosion screening based on moment tensor angular distance. Unpublished report. (LA-UR-22-30001)

**Peer-reviewed*

Granddaughter Radiochronometry for Nuclear Forensics

Joanna Denton
20190565ECR



Nuclear decay chains for (a) uranium-234 and (b) uranium-235 complete with half-lives. Grayed out boxes are no used for radiochronometry. The measured number of atoms for each of the parent, daughter, and granddaughter can be used to calculate the age of interdicted nuclear material such as that shown in the image (1999 Rouse, Bulgaria, seizure). This project aims to improve radiochronometry by incorporating information about the granddaughter.

Project Description

To date there have been more than 2800 cases of nuclear material being found out of regulatory control. The illegal trafficking of such nuclear material poses a serious risk to global safety and security. Once nuclear material is interdicted, the discipline of nuclear forensics, alongside traditional forensics, attempts to identify a source, destination, and suspected use for the materials. The age, of a material, obtained through radiochronometry, is a key predictive signature in a nuclear forensics investigation. Currently, the age of a material can be obtained through parent-daughter radiochronometry. This project aims to add parent-granddaughter radiochronometry to the Laboratory's nuclear forensics toolbox enabling the age of a material to become more tightly constrained. Additionally, the results of this project will shed light on the behavior of uranium decay products during material processing and production. This information can be used as vital reference points for seizures of unknown uranium materials.

Technical Outcomes

This project provided Los Alamos with a granddaughter radiochronometry capability. New data points have been provided for certified reference materials used for quality assurance purposes. Insights have been gained into the behavior of radionuclides during uranium material production.

Publications

Presentation Slides

Denton, J. S., A. M. Wende, M. A. Edwards, M. E. Sanborn, T. M. Kayzar-Boggs, R. R. Foley and R. E. Steiner. Granddaughter Radiochronometry for Nuclear Forensics: Model Ages for Certified Reference Materials and Uranium Samples. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kailua-Kona, Hawaii, United States, 2022-04-03 - 2022-04-03. (LA-UR-22-22911)

Denton, J. S., A. M. Wende, M. A. Edwards, M. E. Sanborn, T. M. Kayzar-Boggs, R. R. Foley and R. E. Steiner. Granddaughter Radiochronometry for Nuclear Forensics: Model Ages for Certified Reference Materials and Uranium Samples. Presented at *CANUKUS Technica Exchange Virtual Meeting*, Los Alamos, New Mexico, United States, 2022-11-15 - 2022-11-15. (LA-UR-22-32390)

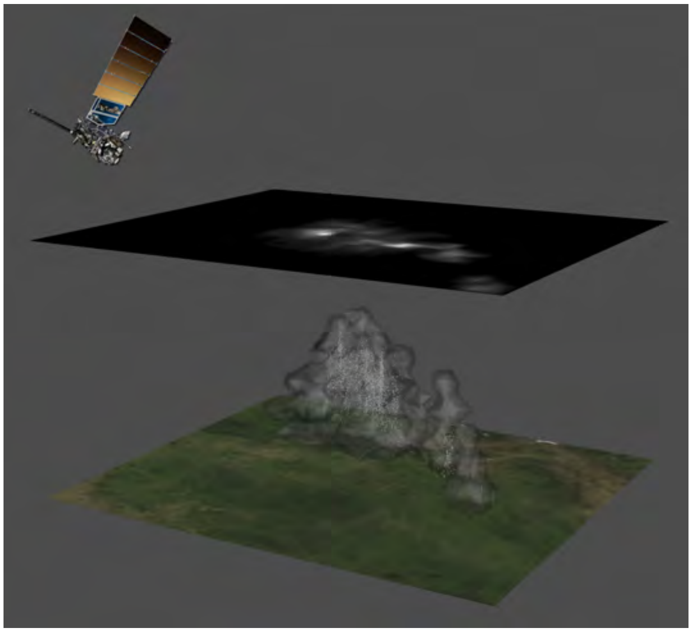
Denton, J. S., A. M. Wende, M. A. Edwards, T. M. Kayzar-Boggs and M. E. Sanborn. Granddaughter-Uranium Radiochronometry. Presented at *VLADIS*, Virtual, New Mexico, United States, 2022-03-29 - 2022-03-29. (LA-UR-22-22912)

Denton, J. S., A. M. Wende, T. M. Kayzar-Boggs, M. A. Edwards and R. E. Steiner. Progress Towards a LANL Granddaughter Radiochronometry Capability. Presented at *BSAP Meeting*, Virtual, New Mexico, United States, 2021-02-09 - 2021-02-09. (LA-UR-21-20996)

**Peer-reviewed*

Using Thundercloud Illumination by Lightning to Understand Optical Signal Propagation in Nature

Michael Peterson
20200529ECR



The clouds surrounding lightning flashes modify the appearance of their optical signals recorded from space. Considering how the clouds are being illuminated by lightning helps us to understand the nature of these modifications, allowing us to make inferences about the lighting source and surrounding thunderclouds. This is demonstrated in this visualization, which takes two-dimensional (2D) lightning observations provided by the Geostationary Lighting Mapper (GLM) on the National Oceanic and Atmospheric Administration's Geostationary Operational Environmental Satellite (GOES-16) (top contour plot) and uses source altitudes inferred from cloud illumination measurements (points) to construct new volumetric imagery of the thunderstorm (3D hull) from the original 2D data.

Project Description

Both nuclear explosions and natural phenomena (lightning, meteor impacts) produce bright flashes of light that can be detected from space. When optical signals have to travel through a cloud to reach the satellite, however, they can be modified by reflection / absorption interactions with raindrops and ice particles. These interactions cause optical space-based sensors like the National Oceanic and Atmospheric Administration's Geostationary Lightning Mapper (GLM) to miss lightning activity in large and dense clouds. They also leave a fingerprint on the optical signals that make it through to the satellite. The United States Department of Energy (DOE) supports development of optical and radio-frequency sensors for nuclear treaty monitoring. Those signals experience these same effects, so using lightning to better understand the propagation effects benefits sensor design and performance assessments in the United Stated Nuclear Detonation Detection System program.

Technical Outcomes

This project was successful in improving our understanding of how optical signals are modified by clouds before reaching on-orbit sensors. Optical lightning measurements were used to investigate cloud structures that are apparent when clouds are illuminated, their evolution over time with the development of the thunderstorm, and implications for on-orbit optical detection. A new three-dimensional volume imaging capability was developed that makes it possible to compare lightning activity and cloud illumination from different vertical levels.

Publications

Journal Articles

*Peterson, M. Holes in Optical Lightning Flashes: Identifying Poorly Transmissive Clouds in Lightning Imager Data. 2021. *Earth and Space Science*. **8** (2): e2020EA001294. (LA-UR-20-22888 DOI: 10.1029/2020EA001294)

*Peterson, M. Modeling the Transmission of Optical Lightning Signals Through Complex 3-D Cloud Scenes. 2020. *Journal of Geophysical Research: Atmospheres*. **125** (23): e2020JD033231. (LA-UR-20-23479 DOI: 10.1029/2020JD033231)

*Peterson, M. FORTE Measurements of Global Optical Lightning Waveforms and Implications for Optical Lightning Detection. 2022. *Earth and Space Science*. **9** (6): e2022EA002280. (LA-UR-21-32433 DOI: 10.1029/2022EA002280)

*Peterson, M. Combined Optical and Radio-Frequency Perspectives on the Time Evolution of Lightning Measured by the FORTE Satellite. 2022. *Earth and Space Science*. **9** (6): e2022EA002281. (LA-UR-22-20047 DOI: 10.1029/2022EA002281)

*M. D. *. B. D. Peterson, M. *. and M. Peterson. A Global LIS/OTD Climatology of Lightning Flash Extent Density. 2021. *Journal of Geophysical Research: Atmospheres*. **126** (8): e2020JD033885. (LA-UR-20-26320 DOI: 10.1029/2020JD033885)

*Peterson, M. J. Where are the Most Extraordinary Lightning Megaflashes in the Americas?. 2020. *Bulletin of the American Meteorological Society*. 1-26. (LA-UR-20-23234 DOI: 10.1175/BAMS-D-20-0178.1)

*Peterson, M. J. The Illumination of Thunderclouds by Lightning: 1. The Extent and Altitude of Optical Lightning Sources. 2022. *Journal of Geophysical Research: Atmospheres*. **127** (1): e2021JD035579. (LA-UR-21-22307 DOI: 10.1029/2021JD035579)

Peterson, M. J. The Illumination of Thunderclouds by Lightning: Part 3: Retrieving Optical Source Altitude. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-21-23257)

*Peterson, M. J., T. J. Lang, T. Logan, C. W. Kiong, M. Gijben, R. Holle, I. Kolmasova, M. Marisaldi, J. Montanya, S. D. Pawar, D. Zhang, M. Brunet and R. S. Cerveny. New WMO Certified Megaflash Lightning Extremes for Flash Distance and Duration Recorded from Space. 2022. *Bulletin of the American Meteorological Society*. **103** (4): 257-261. (LA-UR-21-29056 DOI: 10.1175/BAMS-D-21-0254.1)

Peterson, M. J. and G. Stano. The Hazards Posed by Mesoscale Lightning Megaflashes. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-20-25866)

*Peterson, M., T. E. L. Light and D. Mach. The Illumination of Thunderclouds by Lightning: 2. The Effect of GLM Instrument Threshold on Detection and Clustering. 2022. *Earth and Space Science*. **9** (1): e2021EA001943. (LA-UR-21-22572 DOI: 10.1029/2021EA001943)

*Peterson, M. and D. Mach. The Illumination of Thunderclouds by Lightning: 4. Volumetric Thunderstorm Imagery. 2022. *Earth and Space Science*. **9** (1): e2021EA001945. (LA-UR-21-25408 DOI: 10.1029/2021EA001945)

Presentation Slides

Mach, D., M. J. Peterson and M. Bateman. Current and Future Processing Techniques for Orbital Optical Lightning Sensors. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29634)

Peterson, M. J. Holes in Optical Lightning Flashes: Identifying Poorly-Transmissive Clouds in Lightning Imager Data. . (LA-UR-20-22698)

Peterson, M. J. Modeling Lightning Illuminating Complex 3D Cloud Scenes. . (LA-UR-20-23063)

Peterson, M. J. A CIERRA Gridded Product Climatology for LIS/OTD. . (LA-UR-20-24470)

Peterson, M. J. A New CIERRA Gridded Product Climatology for LIS/OTD. . (LA-UR-20-25628)

Peterson, M. J. GLM Observations of Extraordinary Lightning Including Two New World Lightning Records. Presented at *GLM Science Team Meeting*, Huntsville (Virutal), Alabama, United States, 2020-09-08 - 2020-09-10. (LA-UR-20-26389)

Peterson, M. J. Imaging Thunderclouds with the Geostationary Lightning Mapper. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29389)

Peterson, M. J. The Most Extraordinary Lightning Recorded by Satellites. Presented at *AMS Annual Meeting*, Online, New Mexico, United States, 2021-01-10 - 2021-01-15. (LA-UR-20-30220)

Peterson, M. J. and D. Mach. Documenting Lightning from Space with Optical and Radio-Frequency Sensors. Presented at *URSI_GASS*, Rome, Italy, 2021-08-28 - 2021-09-04. (LA-UR-21-27593)

Peterson, M. J. and D. Mach. Mapping Lightning in Three Dimensions with Optical Space-Based Lightning Imagers. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31100)

Peterson, M. J. and D. Mach. Volumetric Meteorological Imagery from the Geostationary Lightning Mapper. Presented at *102nd Annual Meeting of the American Meteorological Society*, Houston, Texas, United States, 2022-01-23 - 2022-01-27. (LA-UR-21-31446)

Posters

Peterson, M. J. Imaging Thunderclouds with the Lightning Imaging Sensor and Geostationary Lightning Mapper.

Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29572)

Stano, G. and M. J. Peterson. An Investigation of Geostationary Lightning Mapper Flash Extent. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29564)

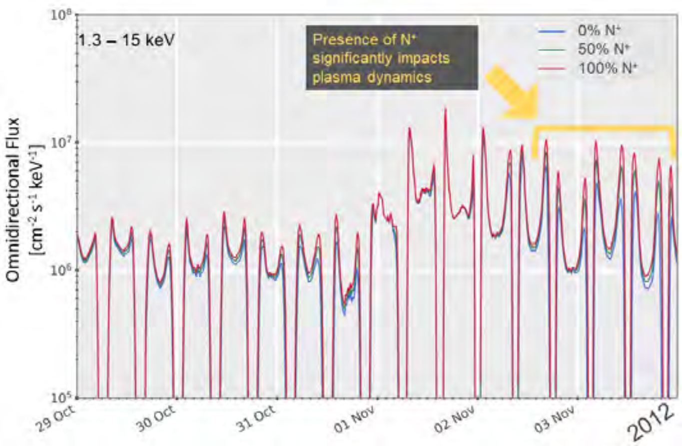
Other

Peterson, M. J. GLM Full Disk Lighting Video. Audio/Visual. (LA-UR-20-23650)

**Peer-reviewed*

Nitrogen: Abundant on Earth and Forgotten in Space

Philip Fernandes
20200580ECR



The dearth of Nitrogen (N+) measurements in space and our poor understanding of differences in plasma processes driven by N+ versus Oxygen (O+) inhibit our ability to predict and characterize natural and man-made events in the near-Earth space environment. Output from RAM-SCB (Ring-current Atmosphere interactions Model with Self-Consistent magnetic field) for plasma with nitrogen abundance 0% (blue), 50% (green), and 100% (red) shows that the measured ion flux can double based on the N+ abundance (yellow region). Development of a low-resource technique for measuring N+ and O+ along with global modeling will enable understanding of the processes in near-Earth space.

Project Description

Few measurements exist of nitrogen ions (N+) in the Earth's space environment, and most are from the 1970s–1990s. Modern literature treats N+ and O+ (oxygen ions) as interchangeable despite numerous measurements and models which show these ions behave very differently in space. Our poor knowledge of the differences in source, transport, and loss of N+ and O + in the space environment hinders our ability to predict space weather, which is important for the Lab's space national security programs. Satellite measurements of O+ are used as a signature of geomagnetic storms: sun-driven disturbances that have broad, deleterious impact on the Nation, including radiation effects on satellites due to enhanced radiation belts, increased ionospheric scintillation that distorts radio, radar, and Global Positioning System (GPS) signals, and geomagnetically induced currents that can disrupt ground-based electrical power grids. Even more fundamental: our lack of knowledge of N+ transport prevents accurate understanding and prediction of the impact of a high-altitude nuclear explosion (HANE) on our space infrastructure, or detection of neighboring and potentially adversarial spacecraft (SDA: space domain awareness). We will develop a low-resource instrument capable of distinguishing N+ from O+, thus enabling addressing of mission-critical background measurements relevant to space weather, HANE, and SDA.

Technical Outcomes

The project successfully addressed the described goals/ objectives. The team analyzed spacecraft data, published two articles and one poster on the importance of nitrogen in near-Earth space, and developed a model of a novel low-resource instrument concept capable of distinguishing nitrogen from oxygen. This promoted community excitement and places Los Alamos in an ideal position to lead an instrument measuring nitrogen in space.

Publications

Journal Articles

Fernandes, P. A., G. L. Delzanno, M. H. Denton, M. G. Henderson, V. K. Jordanova, K. H. Kim, B. A. Larsen, C. A. Maldonado, E. G. D. Reeves, D. B. Reisenfeld and R. M. Skoug. Heavy Ions: Tracers and Drivers of Solar Wind/ Ionosphere/Magnetosphere Coupling. Submitted to *Heliophysics 2050 white paper*. (LA-UR-20-27388)

Vira, A. D., B. A. Larsen, R. M. Skoug and P. A. Fernandes. Bayesian Model for HOPE Mass Spectrometers on Van Allen Probes. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-20-26079)

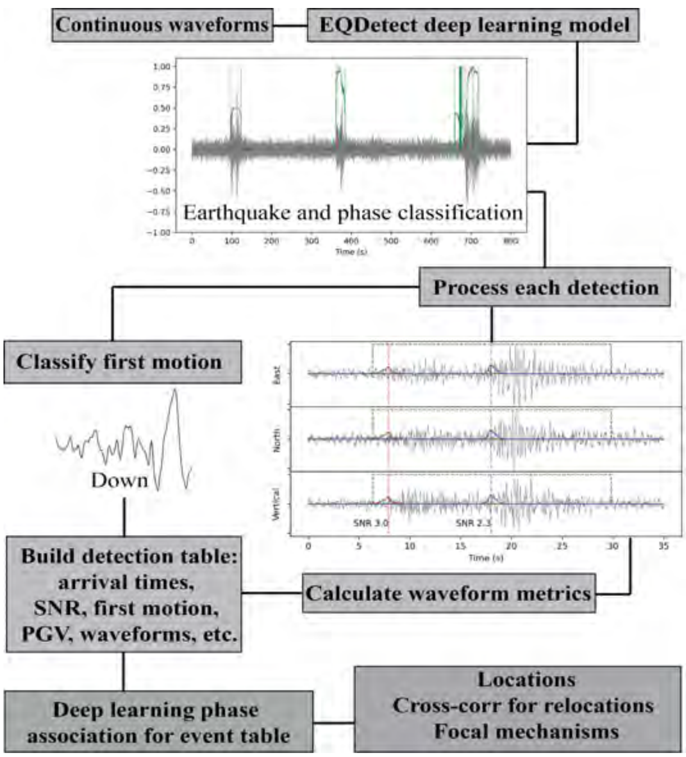
Posters

Fernandes, P. A., G. L. Delzanno, M. H. Denton, M. G. Henderson, V. K. Jordanova, K. H. Kim, B. A. Larsen, C. A. Maldonado, E. G. D. Reeves, D. B. Reisenfeld and R. M. Skoug. Heavy Ions: Tracers and Drivers of Solar Wind/ Ionosphere/Magnetosphere Coupling. Presented at *Heliophysics 2050 Workshop*, Los ALamos, New Mexico, United States, 2021-05-03 - 2021-05-07. (LA-UR-21-25792)

**Peer-reviewed*

The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting

Christopher Johnson
20200681PRD1



Processing workflow to apply continuous waveforms to deep learning models, build an earthquake detection table with waveform metrics, associate phase arrivals into event table, and develop catalog. The earthquake_phase_detection software is adaptable to update the deep learning model and output fields to classify more phase arrivals and classes of environmental noise.

Project Description

The national security challenge the project addresses is earthquake hazard from human-caused or natural earthquakes. The high-level goals of this research are to make dramatic advances in characterizing how earthquakes work during the entire earthquake cycle (from one earthquake to the next), and to attempt to dramatically advance earthquake forecasting—the time, location and magnitude of an earthquake. This work will develop the means to address earthquake hazard associated with energy extraction (geothermal, hydrocarbon) and waste storage (wastewater, carbon dioxide, nuclear). The work could also have significant impact to Ground Based Explosion Monitoring for developing approaches to identify anomalous sources. Although a high-risk research endeavor, the potential life-safety and economic impact of this proposal cannot be overstated. Moreover, this work will have broad impact to nearly all problems where prediction of brittle failure is crucial.

Publications

Journal Articles

Bordelon, M. M., C. P. M. Girod, F. Ronning, J. D. Thompson, C. dela Cruz, S. M. Thomas, E. D. Bauer and P. Rosa. Interwoven atypical quantum states in CeLiBi2. Submitted to *Physical Review B*. (LA-UR-22-30685)

Chen, K., T. Yeh, C. W. Johnson, C. Lin, Y. Lai and M. Shih. Whispering of the city: Characteristics and origin of environmental shaking in the Taipei metropolitan area. Submitted to *Geophysical Research Letters*. (LA-UR-21-20002)

Johnson, C. W., C. L. Hulbert, B. P. G. Rouet-Leduc and P. A. Johnson. Learning the low frequency earthquake daily intensity on the central San Andreas Fault. Submitted to *Geophysical Research Letters*. (LA-UR-20-28772)

Johnson, C. W., N. Lau and A. Borsa. An assessment of GPS velocity uncertainty in California. Submitted to *Earth and Space Science*. (LA-UR-20-29137)

Johnson, C. W. and P. A. Johnson. EQDetect: Earthquake phase arrivals and first motion polarity with deep learning. Submitted to *Journal of Geophysical Research: Earth Surface*. (LA-UR-22-23463)

Johnson, C. W. and P. A. Johnson. Hidden seismic fingerprint predicts ground motions during the 2018 Kilauea collapse sequence. Submitted to *Science*. (LA-UR-23-20248)

*Meng, H., Y. Ben-Zion and C. W. Johnson. Analysis of Seismic Signals Generated by Vehicle Traffic with Application to Derivation of Subsurface Q-Values. 2021. *Seismological Research Letters*. **92** (4): 2354-2363. (LA-UR-20-26366 DOI: 10.1785/0220200457)

Umlaft, J., C. W. Johnson, P. Roux, D. Trugman, A. Lecointre, A. Walperdorf, U. Nanni, F. Gimbert, B. Rouet-Leduc, C. Hulbert and P. A. Johnson. Mapping glacier basal sliding applying machine learning. Submitted to *Earth and Planetary Science Letters*. (LA-UR-23-20247)

Wang, K., C. W. Johnson, K. C. Bennett and P. A. Johnson. Predicting Future Laboratory Fault Friction Through Deep Learning Transformer Models. 2022. *Geophysical Research Letters*. **49** (19): e2022GL098233. (LA-UR-22-20930 DOI: https://doi.org/10.1029/2022GL098233)

*Wang, K., C. W. Johnson, K. C. Bennett and P. A. Johnson. Predicting fault slip via transfer learning. 2021. *Nature Communications*. **12** (1): 7319. (LA-UR-21-26470 DOI: 10.1038/s41467-021-27553-5)

*Xue, L., Y. Fu, C. W. Johnson, J. J. Otero Torres, C. K. Shum and R. B\xc3\xbcrgmann. Seasonal Seismicity in the Lake Biwa Region of Central Japan Moderately Modulated by Lake Water Storage Changes. 2021. *Journal of Geophysical Research: Solid Earth*. **126** (12): e2021JB023301. (LA-UR-21-20003 DOI: 10.1029/2021JB023301)

Reports

Johnson, C. W. and P. A. Johnson. The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting. Unpublished report. (LA-UR-21-25480)

Presentation Slides

Johnson, C. W. Probing fault systems using hydrospheric induced stress modulation. Presented at *GAGE/SAGE 2021 Community Science Workshop*, Online, NM, New Mexico, United States, 2021-08-17 - 2021-08-17. (LA-UR-21-26995)

Johnson, C. W. Characterizing emergent and impulsive non-tectonic signals in seismic waveforms. Presented at *Seismological Society of America Annual Meeting*, Bellevue, Washington, United States, 2022-04-19 - 2022-04-19. (LA-UR-22-23220)

Johnson, C. W. Seismological Society of America Annual Meeting 2022 Workshop: Machine Learning II: Advance your Skills. . (LA-UR-22-23339)

Johnson, C. W., B. P. G. Rouet-Leduc and P. A. Johnson. Testing the ability of machine learning models to predict the timing of seismogenic nucleation. Presented at *AGU Fall Meeting 2020*, Online, NM, New Mexico, United States, 2020-12-07 - 2020-12-07. (LA-UR-20-29569)

Johnson, C. W. and P. A. Johnson. The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting. . (LA-UR-20-30323)

Johnson, C. W. and P. A. Johnson. The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting. . (LA-UR-21-20094)

Johnson, C. W. and P. A. Johnson. Microseismicity Deep Learning Model Developed and Applied to the Central U.S.. Presented at *AGU Fall Meeting 2021*, Online, NM, New Mexico, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31905)

Johnson, C. W. and P. A. Johnson. Anatomy of the seismic wavefield and the search for elusive precursors. . (LA-UR-22-31897)

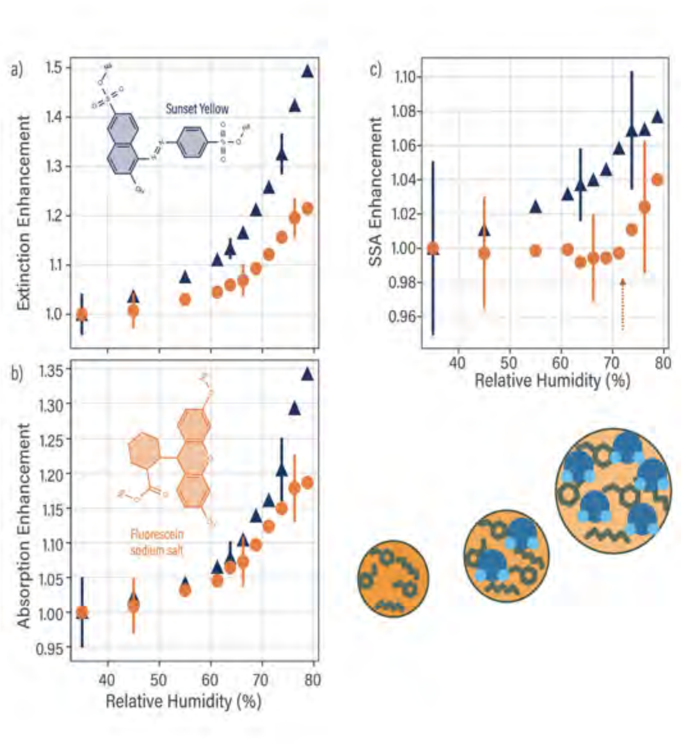
Posters

Johnson, C. W. Identifying weak ground motions to characterize fault zone strain localization. Presented at *SCEC Rupture and Fault Zone Obervartory Workshop*, Online, New Mexico, United States, 2021-04-13 - 2021-04-13. (LA-UR-21-23451)

**Peer-reviewed*

The Next Generation of Aerosol Optical Models: Humidity Dependence and Chemical Processing

Kyle Gorkowski
20200752PRD3



The enhancement in extinction (a), absorption (b) and single scatter albedo (scattering/extinction)(c) as a function of relative humidity for the two aromatic brown carbon mimics measured with our new Humidified- Cavity Attenuated Phase Shift Particle Matter Single Scatter Albedometer (H-CAPS-PMssa) monitor at 450 nanometers.

Project Description

Light absorbing particles from fires and explosions absorb sunlight reducing visibility and climate that can be enhanced if these particles take up water in humid air. The project will perform focused experiments to quantify these optical effects on targeted aerosols and analyze the results for predictive models. The results can be incorporated into atmospheric visibility, air quality, and climate models to improve forecasts for battlefield, wildfire, and climate impact response. It will also improve remote sensing for nuclear forensics and fire predictions on the battlefield. The results also have applications for next-generation photo-voltaic and nanomaterials for energy security.

Publications

Journal Articles

*Gorkowski, K., K. B. Benedict, C. M. Carrico and M. K. Dubey. Complexities in Modeling Organic Aerosol Light Absorption. 2022. *The Journal of Physical Chemistry A*. **126** (29): 4827-4833. (LA-UR-21-32053 DOI: 10.1021/acs.jpca.2c02236)

*Sullivan, R. C., H. Boyer-Chelmo, K. Gorkowski and H. Beydoun. Aerosol Optical Tweezers Elucidate the Chemistry, Acidity, Phase Separations, and Morphology of Atmospheric Microdroplets. 2020. *Accounts of Chemical Research*. **53** (11): 2498-2509. (LA-UR-20-24435 DOI: 10.1021/acs.accounts.0c00407)

Reports

Gorkowski, K. J., S. H. Jordan, K. B. Benedict and M. K. Dubey. A novel approach to characterize the full spectrum and radiative properties of aerosols. Unpublished report. (LA-UR-21-28132)

Presentation Slides

Gorkowski, K. J., A. Rafferty, T. C. Preston, A. Zuend, R. Sullivan, N. Donahue, T. Capek, C. Mazzoleni, C. Carrico, J. E. Lee, A. C. Aiken and M. K. Dubey. One particle at a time: Insights from the Aerosol Optical Tweezers. Presented at *New Mexico Tech Seminar*, Los Alamos, New Mexico, United States, 2020-11-12 - 2020-11-12. (LA-UR-20-29250)

Gorkowski, K. J., A. Rafferty, T. Preston, A. Zuend, R. Sullivan, N. Donahue, T. Capek, C. Mazzoleni, C. Carrico, J. E. Lee, A. C. Aiken and M. K. Dubey. Exploring the outsized role humidity has on aerosol particles: Aerosol Optical Tweezers and Wildfires. Presented at *Georgia Technological University Invited Seminar*, Atlanta, Georgia, United States, 2020-09-24 - 2020-09-24. (LA-UR-20-27412)

Gorkowski, K. J., J. E. Lee, T. Capek, C. Mazzoleni, C. Carrico, A. C. Aiken and M. K. Dubey. Humidity Dependent Absorption Enhancements for Brown Carbon Surrogates. Presented at *American Association for Aerosol Research, Fall Meeting*, online, New Mexico, United States, 2020-10-05 - 2020-10-09. (LA-UR-20-27509)

Gorkowski, K. J., K. B. Benedict, J. E. Lee, A. C. Aiken, C. Carrico, T. Capek and M. K. Dubey. Humidity-Dependent Brown Carbon Light Absorption and Photobleaching: Laboratory and Model Synthesis of Organic Dyes.. Presented at *American Association for Aerosol Research 39th annual conference*, Albuquerque, New Mexico, United States, 2021-10-18 - 2021-10-22. (LA-UR-21-29966)

Gorkowski, K. J., K. B. Benedict, J. E. Lee, A. C. Aiken, C. Carrico and M. K. Dubey. Laboratory and Model Synthesis of Brown Carbon Dyes: Humidity-Dependence and Photobleaching. Presented at *Air and Waste Management Association: Atmospheric Optics: Aerosols, Visibility, and the Radiative Balance*, Bryce Canyon, Utah, United States, 2021-10-04 - 2021-10-08. (LA-UR-21-29546)

Gorkowski, K. J., M. K. Dubey, T. Capek, C. Carrico, K. B. Benedict, J. E. Lee and A. C. Aiken. Observing RH-Dependent Absorbing Aerosol Optics: Gray and Brown Carbon, and TRACER-CAT. Presented at *2021 ARM/ASR PI Meeting*, online, New Mexico, United States, 2021-06-21 - 2021-06-24. (LA-UR-21-25281)

Gorkowski, K. J., S. H. Jordan, K. B. Benedict and M. K. Dubey. A novel approach to characterize the complex refractive index spectrum of organic aerosols. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31762)

Gorkowski, K. J., S. H. Jordan and K. B. Benedict. A new approach to measure the light absorption of aerosols. . (LA-UR-21-27755)

Posters

Gorkowski, K. J., T. Capek, C. M. Carrico, J. E. Lee, A. C. Aiken, C. Mazzoleni and M. K. Dubey. Molecular Foundations of Humidity Dependent Absorption Enhancements by Brown Carbon Surrogates. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-02 - 2020-12-02. (LA-UR-20-29463)

**Peer-reviewed*

Distinguishing Uranium Oxides using Table-Top Extreme Ultraviolet Absorption Spectroscopy to Elucidate Reaction Kinetics and Conglomeration in Uranium-containing Laser Ablation Plasmas

Pamela Bowlan
20210916PRD2

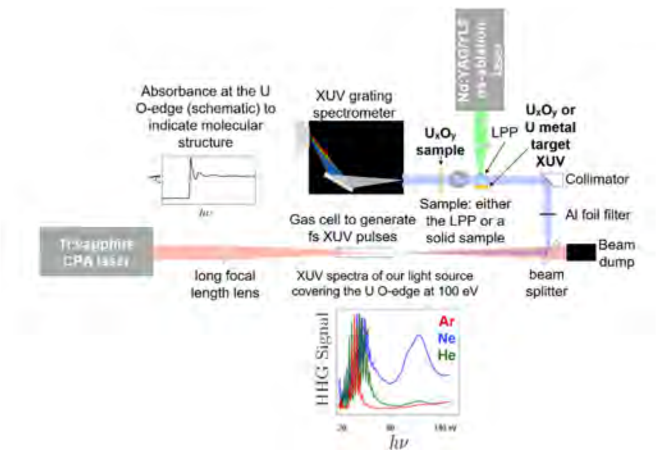


Table-top higher order harmonic generation (HHG) driven by a Ti:sapphire-based chirped pulse amplification (CPA) laser provides an extreme ultraviolet (XUV) source for X-ray absorption near-edge spectroscopy (XANES) to determine the structure of uranium oxides and conglomerates. Three types of uranium oxide (UxOy) samples will be studied: (1) phase-pure UxOy grown via pulsed laser deposition, and (2) UxOy conglomerates formed from nanosecond (ns)-pulsed laser ablation of uranium (U) metal and (3) UxOy conglomerates formed during ns-laser ablation of U metal. Finally, the pulsed XUV source will be used to study the spatiotemporal evolution of gas-phase UxOy in a ns-laser-produced plasma (LPP) in situ.

Project Description

Forensics tools are needed for analyzing nuclear materials or debris. The commonly used visible and infrared spectroscopic tools have proven incapable of distinguishing different uranium oxides compounds. X-ray spectroscopy has proven to be a reliable approach for identifying uranium oxides, but typically requires taking these hazardous materials to synchrotrons. We propose instead to use a table top extreme ultraviolet (XUV) light source to provide the needed distinct signatures. Taking advantage of Los Alamos National Laboratory collaborators capabilities to grow high quality Uranium Oxide (UxOy) single crystal thin films, we will build a small library of the XUV signatures. As a next step, the same laser which we use to produce the XUV light will be used to create a uranium plasma, so that with the XUV spectroscopy, we can both produce and measure signatures of the UxOy conglomerates and also time-resolve their growth. This is highly relevant for mission relevant for developing novel signatures for nuclear forensics and for analyzing nuclear debris. The general concept to do work that is typically done at x-ray synchrotron at a table-top source at Los Alamos, has many potential mission relevant applications in forensics of other hazardous materials or materials in extreme conditions.

Publications

Reports

Skrodzki, P. J. and P. R. Bowlan. Distinguishing uranium oxides using table-top extreme ultraviolet absorption spectroscopy to elucidate reaction kinetics and conglomeration in U-containing laser ablation plasmas. Unpublished report. (LA-UR-22-27646)

Presentation Slides

Skrodzki, P. J. Standoff laser-based optical spectroscopy of uranium enabled by ultrafast laser filamentation in air. . (LA-UR-21-28434)

**Peer-reviewed*

Planetary Acoustics: A Brand New Sense with which to Explore Atmospheres in our Solar System

Nina Lanza
20210960PRD3

The SuperCam microphone on board the Perseverance rover recorded the first sounds on another planet in 2021. It is being used to understand sound propagation in a very different atmosphere, both in terms of pressure and composition, than on Earth. The microphone records sounds of the wind (providing new information on Mars atmospheric turbulence), the flights of the Ingenuity helicopter, and laser plasmas produced on nearby rocks. The latter provides information on rock physical properties (hardness, surface coatings) as well as information on atmospheric thermal gradients between the source and the receiver.

Project Description

We plan to study of the acoustic properties of Mars with a microphone on board the Perseverance rover, and also study a broad range of planetary atmospheres in the laboratory, including variations in composition, pressure, and temperature. This experimental work will be supported by theoretical developments in sound propagation in atmospheres with these properties. Our studies will aid in the design of a new microphone-based instrument concept for planetary exploration, especially for Venus and Titan. For these planets, theoretical models, sound propagation, attenuation and noise sources will be improved. This work has side benefits in using acoustic signals for remote detection of events (including rocket launches, overflights, explosions) on Earth.

Publications

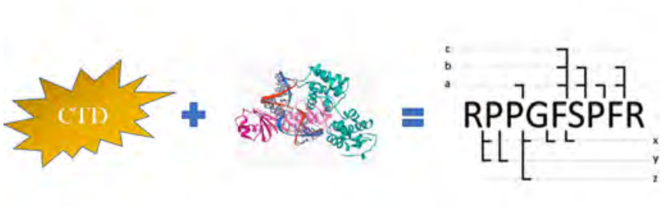
Journal Articles

Chide, B., T. Bertrand, R. D. Lorenz, A. Munguira, R. Hueso, A. S\xc3\xa1nchez-Lavega, G. Martinez, A. Spiga, X. Jacob, M. de la Torre Juarez, M. T. Lemmon, D. Banfield, C. E. Newman, N. Murdoch, A. Stott, D. Vi\xc3\xbadez-Moreiras, J. Pla-Garcia, C. Larmat, N. L. Lanza, J. A. Rodr\xc3\xadguez-Manfredi and R. C. Wiens. Acoustics Reveals Short-Term Air Temperature Fluctuations Near Mars' Surface. 2022. *Geophysical Research Letters*. **49** (21). (LA-UR-22-31591 DOI: 10.1029/2022GL100333)

**Peer-reviewed*

Application of Charge Transfer Dissociation to Omics and Chemical, Biological, Radiological, Nuclear, and high yield Explosives Threats

Trevor Glaros
20220794PRD2



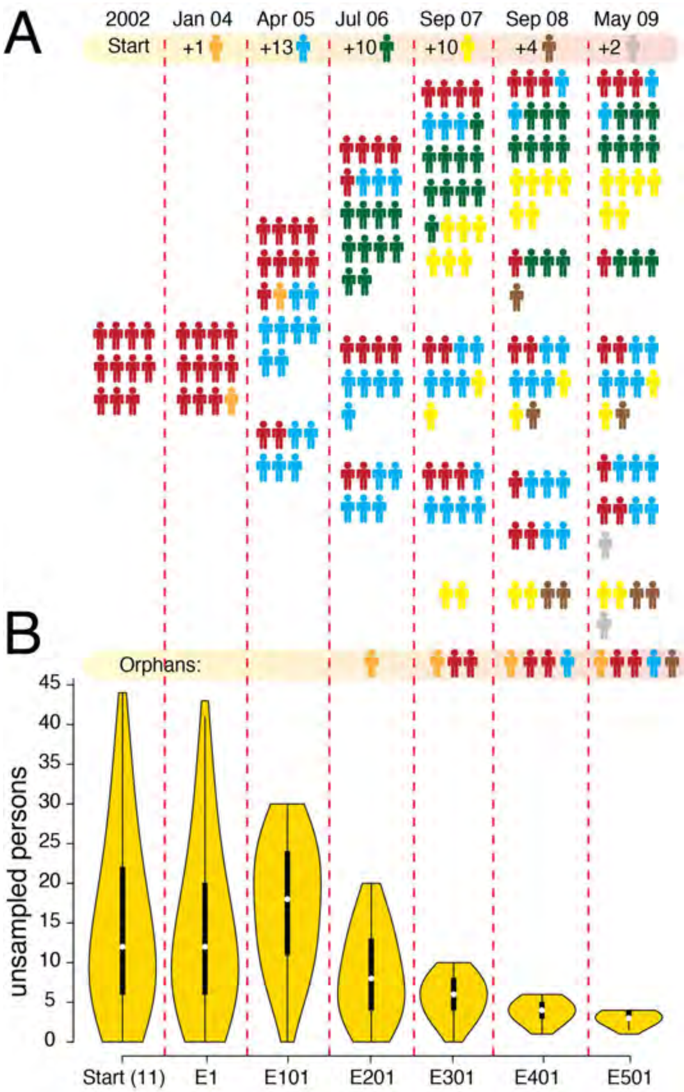
An ion trap mass spectrometer will be modified to enable a state-of-the-art fragmentation technique called charge transfer dissociation (CTD) to generate deeper structural information that contains more granularity compared to traditional fragmentation techniques used in proteomic workflows.

Project Description

The deep characterization of living systems is inherently linked to the integration of several 'omics' data streams. Mass spectrometry-based omics is central to several of these techniques including proteomics, metabolomics, and lipidomics (i.e. the characterization of proteins, metabolites, and lipids, respectively). This research aims to assess a new mass spectrometry fragmentation technique, charge transfer dissociation (CTD), which has shown promise in terms of revealing key structural information needed to assign molecular structure which is currently not possible using existing commercialized fragmentation strategies (e.g. collision induced dissociation, (CID)). If successful, this strategy would advance the fields of metabolomics and lipidomics by at least a decade by enabling the bioinformatic determination of structure.

Improving Public Health by Linking Virus Genetic Evolution and Epidemic Spread

Arshan Nasir
20180751PRD3



Tracking virus spread in human populations is an enormous challenge. We have developed a computational framework that splits HIV-1 phylogenies into clusters linked by virus transmission and then updates those clusters every time new sequences are added. The panel A shows the growth of an initial cluster of 11 individuals who infected each other via needle sharing to 51 over ~7 years. In parallel, panel B estimates the number of unsampled individuals who may be involved in the outbreak at each time point. The framework allows real-time tracking of virus spread, along with estimating the success of contact tracing efforts.

Project Description

This project aims to develop models, methods, and applications based on the basic evolutionary biology of human viruses to better understand the epidemiology of human viral diseases and, ultimately to help intervene to reduce the burden of disease. Using public health data, including thousands of human immunodeficiency virus (HIV) sequences sampled from real populations, we will develop a computational framework to routinely retrieve virus sequence data (and associated metadata) from public health surveillance systems, apply standard and novel genetics and epidemiological models, and produce automated reports of HIV evolution and spread. This project ties in with the Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) National Security mission of forecasting and predicting biological threats. We focus specifically on the US HIV epidemic, working togheter with the Colorado and Michigan health departments, but our general framework will also be useful, with adaptations, in preventing other pathogen threats, such as Avian Flu, Ebola, Dengue, Zika and other rapidly evolving pathogens. Thus, this project strongly ties in with 'Pathogen Detection and Countermeasures' as well as 'Information Collection, Surveillance, and Reconnaissance' and 'Non-Nuclear Forensics' (as we will reconstruct the hidden who-infected-whom network).

Technical Outcomes

The project developed computational tools based on the evolutionary biology of Human Immunodeficiency Virus-1 (HIV-1), the most common type of HIV virus, to better understand the epidemic spread of HIV-1. The team expects that the developed HIV surveillance framework will be used in real world HIV (and other pathogens) epidemic tracking and prevention. This will put Los Alamos National Laboratory at the forefront of eliminating the HIV epidemic from the United States.

Publications

*Peer-reviewed

Journal Articles

*Bokhari, R. H., N. Amirjan, H. Jeong, K. M. Kim, G. Caetano-Anollés and A. Nasir. Bacterial Origin and Reductive Evolution of the CPR Group. 2020. *Genome Biology and Evolution*. **12** (3): 103-121. (LA-UR-19-24949 DOI: 10.1093/gbe/evaa024)

*Hwang, K., H. Choe, A. Nasir and K. M. Kim. Complete genome of Polaromonas vacuolata KCTC 22033T isolated from beneath Antarctic Sea ice. 2021. *Marine Genomics*. **55**: 100790. (LA-UR-20-23340 DOI: 10.1016/j.margen.2020.100790)

*Mughal, F., A. Nasir and G. Caetano-Anollés. The origin and evolution of viruses inferred from fold family structure. 2020. *Archives of Virology*. **165** (10): 2177-2191. (LA-UR-20-23821 DOI: 10.1007/s00705-020-04724-1)

Nasir, A. Genetic Promiscuity in the Human Microbiome. Submitted to *Science*. (LA-UR-20-20701)

*Nasir, A., E. Romero-Severson and J. Claverie. Investigating the Concept and Origin of Viruses. 2020. *Trends in Microbiology*. **28** (12): 959-967. (LA-UR-20-24424 DOI: 10.1016/j.tim.2020.08.003)

*Nasir, A., F. Mughal and G. Caetano-Anolles. The tree of life describes a tripartite cellular world. 2021. *BioEssays*. **43** (6): 2000343. (LA-UR-20-30493 DOI: 10.1002/bies.202000343)

*Nasir, A., G. Caetano-Anollés and J. Claverie. Editorial: Viruses, Genetic Exchange, and the Tree of Life. 2019. *Frontiers in Microbiology*. **10**: 2782. (LA-UR-19-28355 DOI: 10.3389/fmicb.2019.02782)

*Nasir, A., M. Dimitrijevic, E. Romero-Severson and T. Leitner. Large Evolutionary Rate Heterogeneity among and within HIV-1 Subtypes and CRFs. 2021. *Viruses*. **13** (9): 1689. (LA-UR-21-28214 DOI: 10.3390/v13091689)

*Romero-Severson, E., A. Nasir and T. Leitner. What Should Health Departments Do with HIV Sequence Data?. 2020. *Viruses*. **12** (9): 1018. (LA-UR-20-25996 DOI: 10.3390/v12091018)

Books/Chapters

Nasir, A. and G. Caetano-Anolles. An early cellular origin of viruses. (LA-UR-19-24950)

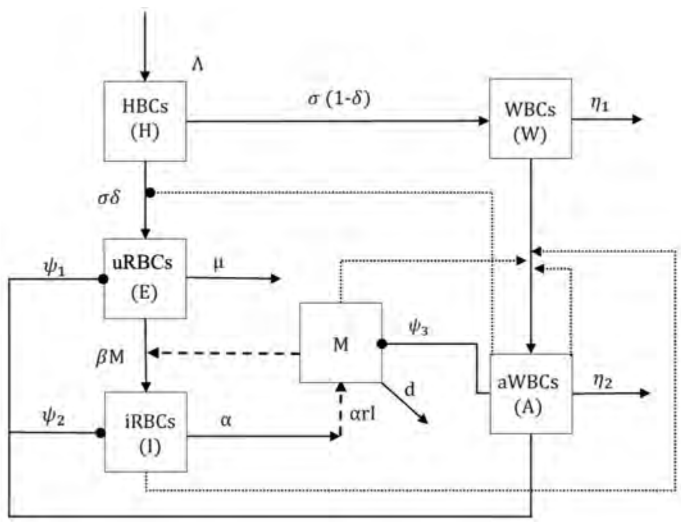
Posters

Goldberg, E. E. Viral Modeling. . (LA-UR-20-26632)

Nasir, A., T. K. Leitner and E. Romero-Severson. Improving Public Health by Linking HIV Genetic Evolution and Epidemic Spread. Presented at *Sandia National Lab's Annual Postdoc Technical Showcase*, Albuquerque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-32531)

Disease Outcome Analysis for Improved Disease Interventions

Paul Fenimore
20190618PRD1



*Flow diagram for malarial anemia: Hematopoietic blood cells (H) are produced at rate Lambda, differentiate into erythrocytes (E) at rate sigma*delta or white blood cells (WBCs) (W) at rate sigma*(1-delta). E die at rate mu, are invaded by free merocytes (M) at rate beta*M or are phagocytized at rate Psi_1. iRBCs (I) are disrupted at a constant rate alpha, realise r new M, or are phagocytized at rate Psi_2. M die at rate d or are engulfed at rate Psi_3. Activated WBCs (A) inhibit erythropoiesis and die at rate nu_2. W is activated by M, I, and A and die at rate nu_1.*

Project Description

This project addresses the need for radically improved multiplexing of both biothreat agent detection schemes and disease marker measurements (biothreat detection needs are exemplified by desired improvements to the Department of Homeland Security's Biowatch program). Improved instrumentation should address both problems. Quanlitatively better data is expected to lead to important advances in our analysis of multiple markers found in serious disease states and complex biothreat monitoring samples.

Technical Outcomes

The project has made substantial progress understanding the genetic factors that predispose some people to severe malarial anemia by examining the genetic sequence information (haplotype). This is an important and novel contribution made in collaboration with Prof. DJ Perkin, University of New Mexico. The microfluidic device has been improved even with substantial delays during the pandemic. Nine colors are now possible, and a conference proceedings paper is in-press.

Publications

Presentation Slides

Fenimore, P. W., G. C. Mcmahon, K. M. Wilding and J. R. Mourant. Microfluidic Spectral Flow Cytometry. Presented at *DTRA CBDS+T*, San Francisco, California, United States, 2022-12-06 - 2022-12-09. (LA-UR-23-20500)

Mcmahon, G. C., K. M. Wilding, C. K. Sanders, P. W. Fenimore, D. J. Perkins and J. R. Mourant. Proof of concept for microfluidic spectral flow cytometry. Presented at *International Society for Optics and Photonics (SPIE) Optics and Photonics Conference*, San Francisco, California, United States, 2023-01-28 - 2023-02-02. (LA-UR-23-20790)

**Peer-reviewed*

Smart Mobile Sensor Platform Development for Radiological Mapping of Large-Scale Areas

Tony Shin
20190625PRD2

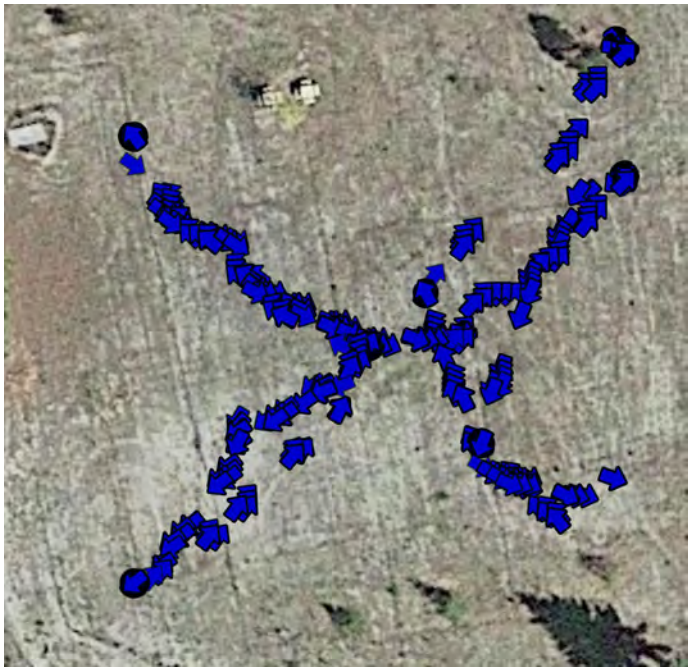


Image of field trial for the unmanned ground vehicle (UGV). Way points were set to the northwest, northeast, southwest, and southeast corner of the field. Plotted in this image is the latitude-longitude readings sent back to the central computer from the UGV global positioning system (GPS). This project aims to develop a smart mobile sensor platform composed of several drones equipped with low-cost radiation sensors to develop a network of detectors that can efficiently survey and create high-fidelity radiological maps of large-scale areas.

Project Description

With the recent developments in drone technology and relatively low-cost radiation sensors (e.g., neutron and gamma-ray sensitive sensors) coupled with well-established statistical techniques, it is possible to implement an intelligent mobile sensor platform that exhibits an active learning methodology through continuous real-time observations of radiological signatures. We propose to develop a smart mobile sensor platform composed of several drones equipped with low-cost radiation sensors to develop a network of detectors that can efficiently survey and create high-fidelity radiological maps of large-scale areas.

This work will demonstrate the potential benefits of utilizing technological advancements in drone technology and low-cost radiation sensors in conjunction with advanced active learning algorithms for radiological mapping of large-scale areas. It will demonstrate how the advanced active learning framework can be developed to ultimately improve on the speed and accuracy of the results. While this research will help improve on current radiological mapping capabilities, it will more generally explore how active learning algorithms can improve any decision making process, thus providing a versatile extension to other fields of interest.

Technical Outcomes

This project developed a framework for a dynamic and recursive optimal motion planning algorithm that utilizes readily available detector data. The algorithm utilizes Gaussian Process Regression models in conjunction with a newly developed prediction-difference mapping routine to improve on the speed of reaching a convergent radiation map compared to the traditional uniform survey routine. The technical outcomes of this work can be extended to any other type of sensor within a mobile sensing platform.

Publications

Journal Articles

*Shin, T. H., D. T. Wakeford and S. F. Nowicki. Multi-Sensor Optimal Motion Planning for Radiological Contamination Surveys by Using Prediction-Difference Maps. 2022. *Applied Sciences*. **12** (11): 5627. (LA-UR-20-26153 DOI: 10.3390/app12115627)

Reports

Raji, D. M. and T. H. S. Shin. Smart Mobile Sensor Platform for Radiation Contamination Mapping of Large-Scale Areas: Algorithmic and Field-Testing Considerations. Unpublished report. (LA-UR-22-30588)

Presentation Slides

Raji, D. M. Applied Multi-Objective Modelling & Optimization. . (LA-UR-22-29551)

Raji, D. M., T. H. S. Shin and W. P. Ford. Autonomous Multi-Robot Radioactive Contamination Mapping. Presented at *NSSC-LANL Keepin Nonproliferation Science Summer Program Student Lightning Presentations*, Los Alamos, New Mexico, United States, 2022-08-10 - 2022-08-10. (LA-UR-22-28301)

S. Shin, T. H. Gaussian process regression for radiological contamination mapping. . (LA-UR-21-20338)

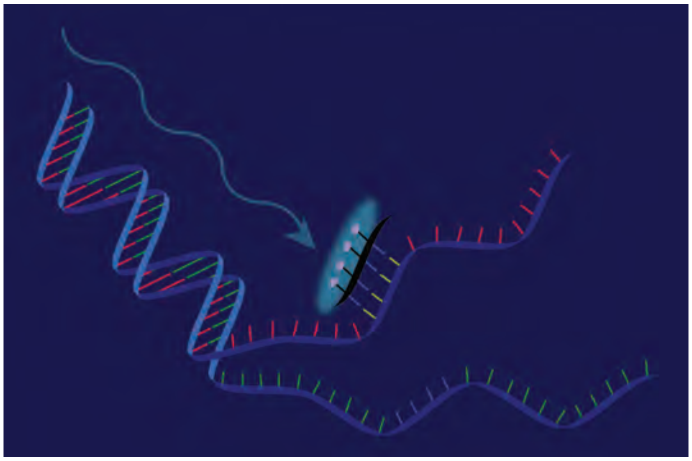
S. Shin, T. H. Gaussian process regression for radiological contamination mapping Applied to optimal motion planning for mobile sensor platforms. . (LA-UR-21-29400)

S. Shin, T. H. and S. F. Nowicki. Smart Mobile Sensor Platform Development for Radiological Mapping of Large-scale Areas. . (LA-UR-21-20339)

**Peer-reviewed*

Superradiant RNA for Single Molecule In-Vivo Fluorescence Microscopy

Murray Wolinsky
20200774PRD4



Conversion of DNA into RNA, or "transcription," is the basis of genetic expression in all living organisms. Though fluorescent molecules are powerful reporters for similar biological processes, the use of these molecules for transcription is plagued by very low signal-to-noise, as the signal from a single gene is drowned out by a sea of fluorescently-labeled nucleotides needed for living systems to synthesize RNA. In this project, an alternative route is proposed where fluorescent molecules are electronically coupled to each other to form "J-aggregates" that that be selectively excited in the context of transcription.

Project Description

Understanding the genetic information encoded in deoxyribonucleic acid (DNA) has been increasing so rapidly that anyone can now sequence their genome and find potential markers for disease. However, we need a way to watch what our cells are doing in real time, where messages from the genome in the form of ribonucleic acid (RNA) are constantly changing. This project seeks to use aggregated groups of molecules assembled onto RNA as "addresses" for certain genes. These aggregates have optical properties that will allow them to be singled out in the complex environment of a cell. If successful, this project will produce a platform for establishing causal links between certain stimuli (e.g. pathogens, pharmaceuticals) and genetic responses, with the eventual goal of being able to predict a response on an individual level. This has wide-ranging implications for the development of medical treatments and response to biosecurity threats. For example, in the current coronavirus (COVID-19) pandemic, a small part of the population has a severe, fatal response to the virus, while the vast majority of the population has a mild response—we currently don't understand why this is, what if we could predict who will have a severe response and why ahead of time?

Technical Outcomes

The project succeeded in developing methods of fluorescently labelling biomolecules. The project developed the approach of using biarsenical dyes to label poly-uridine motifs. Deoxyribonucleic acid (DNA) structures that modulate Cyanine 5 (Cy5) fluorescence intensity through insertion of adenine bases were identified. These structures simultaneously provide photophysical predictability and tunability. This approach improves existing cyanine dyes. Work on fluorescence resonance energy transfer (FRET) gates may prove to be important in enabling future synthetic biology applications.

Publications

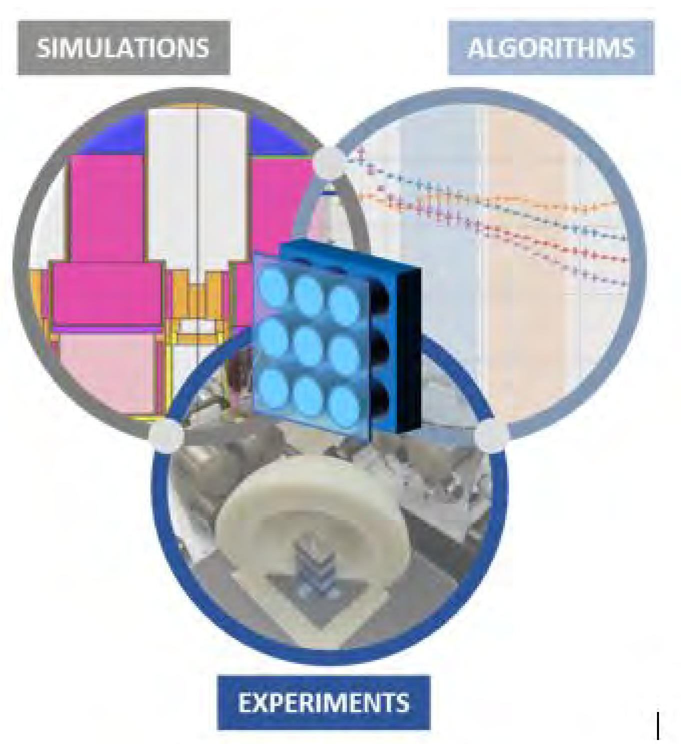
Journal Articles

*Pace, N. A., S. P. Hennelly and P. M. Goodwin. Immobilization of Cyanines in DNA Produces Systematic Increases in Fluorescence Intensity. 2021. *The Journal of Physical Chemistry Letters*. **12** (37): 8963-8971. (LA-UR-21-25758 DOI: 10.1021/acs.jpclett.1c02022)

**Peer-reviewed*

Neutron Spectroscopy for Nuclear Emergency Response Applications

Theresa Cutler
20210548MFR



Nuclear emergency responders require multiple diagnostic tools to reverse-engineer a potential threat item. Neutron energy spectra offer an under-utilized passive signature that can help reduce degeneracies and contribute to render-safe decisions. The designed system must be climate stable, robust, able to penetrate heavy shielding, and easy to operate. This LDRD project combines these highly diverse criteria into a prototype fieldable system also relying on simulations and robust algorithms.

Project Description

The nuclear emergency response mission may require disablement of a nuclear explosive device constructed and placed by an adversary. In order to render the device inoperable, its design must be understood. A combination of passive radiation signatures is used to reverse-engineer the design. Some plausible designs with complex neutron source terms have significant degeneracies in solution space, making absolute determination difficult and untimely. Neutron spectroscopy makes use of a passive signature that is rich with valuable information; however, no tool currently available makes use of this signature. We seek to develop such a tool and determine whether it can be a valuable addition to the toolkit. Our early work shows considerable promise. In Phase 1 we demonstrated the basic physics, interpretation of the raw signal, and signature penetrability through shielding. In Phase 2 we will optimize and ruggedize the system, including replacement of the liquid detector material with a more stable alternative, and we will test against realistic threat designs constructed in a Category-1 nuclear facility in Nevada.

Publications

Reports

Borgwardt, T. C., T. E. Cutler, K. Smith, K. D. Bartlett, C. R. Bates, K. C. Meierbachtol, D. J. Mercer, T. H. S. Shin and R. A. J. Weldon. Neutron Spectroscopy for NER Applications. Unpublished report. (LA-CP-21-20632)

Posters

Cutler, T. E., T. C. Borgwardt and K. Smith. Neutron Spectroscopy for NER Applications. . (LA-UR-21-25477)

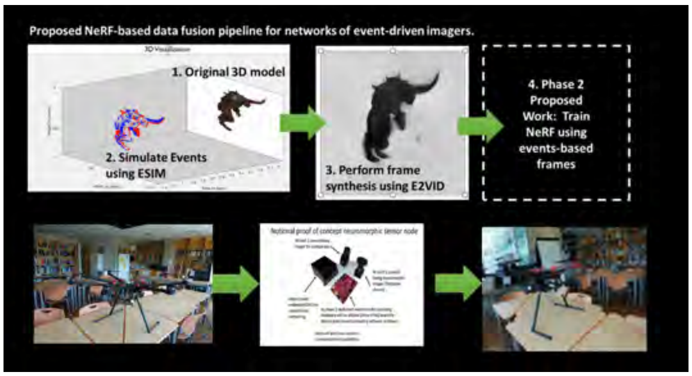
Perello Izaguirre, J. F., T. E. Cutler, T. H. S. Shin, K. D. Bartlett, T. C. Borgwardt, C. R. Bates, D. T. Beckman, D. K. Hemsing, D. J. Mercer and K. Smith. Neutron Spectroscopy for Nuclear Emergency Response Applications. Presented at *Nuclear Particle Futures Capability Review*, Los Alamos, New Mexico, United States, 2023-04-25 - 2023-04-27. (LA-UR-23-23342)

Perello Izaguirre, J. F., T. H. S. Shin, K. D. Bartlett, T. C. Borgwardt, T. E. Cutler, D. J. Mercer and K. Smith. Development of a Portable Organic Glass Neutron Spectrometer. Presented at *Scint 2022*, Santa Fe, New Mexico, United States, 2022-09-19 - 2022-09-23. (LA-UR-22-29490)

**Peer-reviewed*

Neural Radiance Field-Based Data Fusion Across Neuromorphic Imager Arrays for Sky Situational Awareness

David Mascarenas
20220494MFR



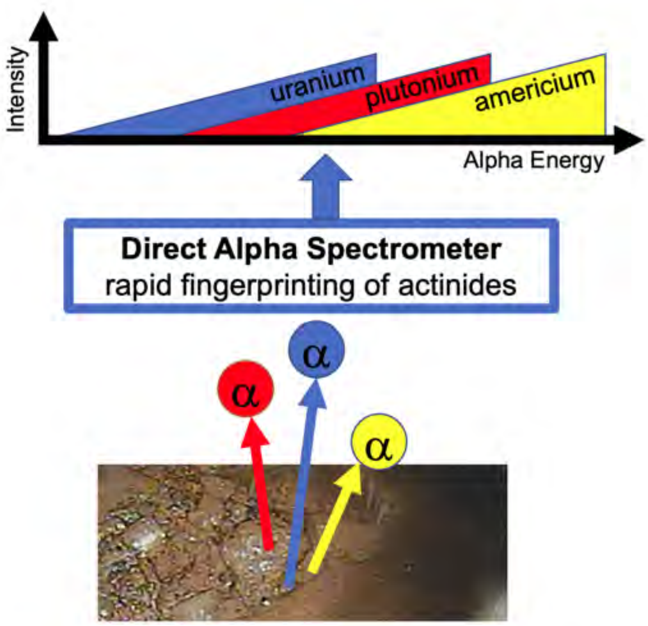
This project aims to develop a neural radiance field-based data fusion pipeline. This computational pipeline is applicable to the sky situational awareness problem which involves tracking and characterizing high-performance drones using a distributed networks of neuromorphic imagers. The project team will also develop visualization techniques based on the view synthesis capabilities of neural radiance field techniques that will allow decision makers to observe an object flying through the sky overserved by the sensors such that they can get a rotatable view of the object.

Project Description

Rapidly advancing drone technology represents both a physical and intelligence threat to troops, airports, critical infrastructure, ships, vehicles, and individuals. As the speed, performance, intelligence, and swarm capabilities of drones continues to increase there will be an increased need to reliably detect the presence of these drones in order to alert vulnerable assets to the danger and to respond appropriately. The challenge with the use of conventional imagers for detecting and characterizing high performance drones is that it would need a very high frame rate to avoid motion blur effects. High frame rates leads to increased power consumption, increased memory requirements, and increased computing resources. In contrast, neuromorphic event-based imagers only detect and report changes in a scene so memory and computing requirements are greatly decreased. Neuromorphic imagers are able to adapt to changing lighting conditions, and have very low-latency. Considering the speed of sound is 343 meters per second, it is unlikely that any drone will be able to out-run the sub 0.1 millisecond latency performance of current event driven imagers in the foreseeable future. At the completion of the first phase of this work the team will demonstrate the capability of using neuromorphic event-driven imagers for high-performance sky situational awareness.

Field-Deployable Alpha Spectrometer for Rapid Fingerprinting of Actinides in Nuclear Accident Scenarios

Mark Croce
20220498MFR



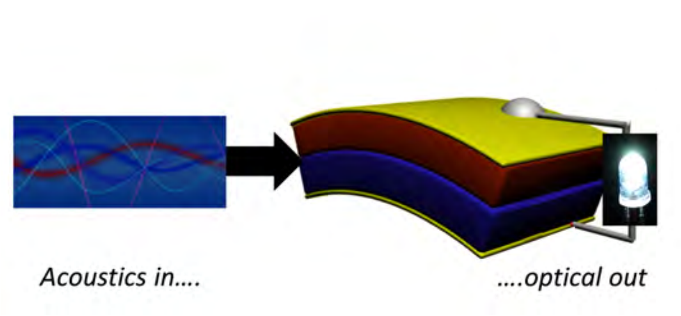
Researchers at Los Alamos National Laboratory are developing the first field-deployable alpha spectrometer to directly determine plutonium, uranium, and other actinide content in nearly any material or debris encountered in field operations for nuclear emergency response, nuclear nonproliferation, and nuclear safeguards. The novel instrument design is expected to provide rapid "fingerprinting" of fissile content in complex materials like spent nuclear fuel (lower image: melted nuclear fuel from Unit 2 Fukushima Dai-Ichi. Credit: TEPCO via Associated Press).

Project Description

We will develop the first field-deployable alpha spectrometer to directly determine plutonium, uranium, and other actinide content in nearly any material or debris encountered in field operations for nuclear emergency response, nuclear nonproliferation, and nuclear safeguards. Alpha spectroscopy in the field is an unresolved problem despite it being a valuable tool in the laboratory for quantifying fissile nuclides such as plutonium (Pu)-239 and uranium (U)-235 to understand a material's history, origin, and intended use. Nuclear emergency response field operations require rapid answers to questions like "How much plutonium is in released spent nuclear fuel?" and "Which fuel assembly has failed?" for which rapid fingerprinting of actinides with our field-deployable alpha spectrometer will be a uniquely valuable tool. Our approach relies on the physical separation in the detector of alpha particles that come from fissile nuclides from interfering radiation, rather than the traditional laboratory approach that requires chemical separations.

Creation of an Acoustic-Optical Transducer

Amanda Graff
20220503MFR



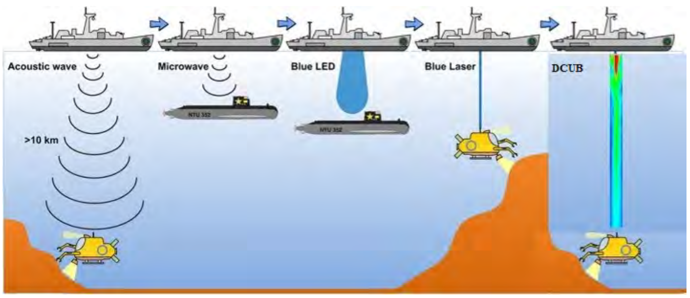
The transformation of acoustic signals into optical signals could open new avenues for remote sensing, nuclear nonproliferation, and intelligence activities. The acoustic-optical transducer (AOT) will demonstrate a new approach to transform vibrations into optical signals that can be leveraged by remote sensing approaches. Because the AOT exploits the triboelectric effect, it can be portable and self-powering. Figure adapted from Wang et al, "Triboelectric nanogenerators as flexible power sources" npj Flex Electron 2017, 1, 10.

Project Description

The interpretation of acoustic signals from remote objects has broad application in global security endeavors. The project team will develop an acoustic-optical transducer (AOT) that converts acoustic signals into optical signals. The final device will be relevant to the remote sensing community.

Unmanned Underwater Vehicles (UUV) Detection using a Highly Directional Collimated Low Frequency Ultrasonic Beam (DCUB)

Eric Davis
20220509MFR



Comparison of the highly Directional Collimated Ultrasonic Beam (DCUB) source versus other methods for UUV detection. Existing methods either have insufficient range, low resolution, or do not function in shallow water. DCUB is capable of deep depth penetration, while maintaining the resolution and collimation needed to detect the small UUVs that are highly illusive to current techniques. Image adapted from Wu et al. (DOI: 10.1038/srep40480) to reflect the main feature of our approach.

Project Description

Currently, Unmanned Underwater Vehicle (UUV) detection in seawater remains a hot topic of research due to the capability of UUVs to inflict damage. Currently, there exists no satisfactory technique that can detect small UUVs at distances long enough to be operationally useful. The highly Directional Collimated Low Frequency Ultrasonic Beam (DCUB) is an acoustic source that aims to provide high resolution imaging at long range through difficult underwater conditions. Through the use of a highly collimated low-frequency source, long range and high resolution can both be realized by one acoustic source. This technology will bridge the gap between low-range, high-resolution technologies and high-range, low-resolution technologies, adding critical detection capability for emerging threats. This fits well into the Global Security mission of “non-traditional threat deterrence” as this technology is a novel sensing platform that will enable detection of hostile UUVs, whose small sizes make them elusive to traditional detection techniques.

Publications

Presentation Slides

Davis, E. S., P. Vakhlamov, C. A. Chavez and C. Pantea. Underwater Object Detection Using a Directional Collimated Low Frequency Ultrasonic Beam (DCUB). Presented at *2022 IEEE IUS*, Venice, Italy, 2022-10-10 - 2022-10-13. (LA-UR-22-29697)

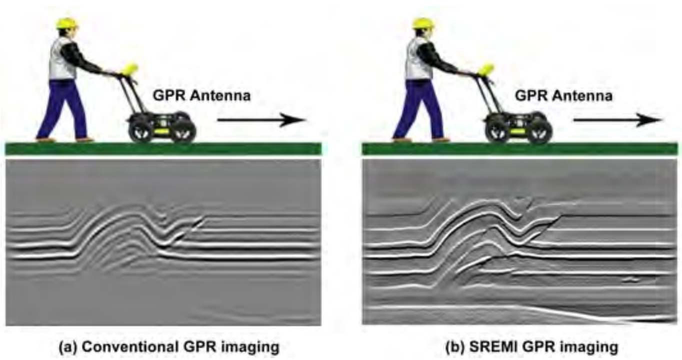
Posters

Davis, E. S., C. Pantea, P. Vakhlamov and C. A. Chavez. Underwater Object Detection Using a Directional Collimated Low Frequency Ultrasonic Beam (DCUB). Presented at *IEEE IUS 2022*, Venice, Italy, 2022-10-10 - 2022-10-13. (LA-UR-22-29306)

**Peer-reviewed*

SREMI: Super-Resolution Electromagnetic Imaging for Near-Surface Target Sensing

Kai Gao
20220484MFR



Panels (a) and (b) display the near-surface structural images produced using conventional GPR imaging and our SREMI GPR imaging techniques, respectively. The goal as well as the most distinct feature of our SREMI GPR imaging technique is to provide a structural image with significantly improved resolution using the same GPR data compared with conventional GPR imaging techniques, to support time-sensitive security applications.

Project Description

Man-made buried objects, such as undetonated ordnance, tunnels, and unmarked pipelines, may post critical threats in battlefields and other security-related field environments. Ground Penetrating Radar (GPR) measurements do not require direct coupling with subsurface, therefore can be collected using remotely-operated rovers or drones, making GPR well-suited for threat detection in high-risk environments. However, the near-surface environment can be highly complex and attenuating, therefore imaging deeper while imaging clearer is usually not simultaneously possible even with current best GPR technique. This work aims at imaging deeper and imaging clearer simultaneously by developing and validating a novel GPR-based super-resolution electromagnetic-wave imaging (SREMI) technique for near-surface target sensing. This research will push the technical boundary for GPR sensing in time-sensitive security applications, and build a SREMI-based near-surface target sensing capability for Los Alamos National Laboratory, Department of Energy, and the National Nuclear Security Administration. The results of this research can be leveraged in many scientific, civil or security-related applications, ranging from geology, non-destructive evaluation, to planetary sciences. For instance, equipped with airborne mobility, our proposed technique can image in real-time large area of forest and mountains that traditionally require costly seismic station installation; it can serve as the next-generation near-surface imaging module for United States planetary rover missions on the Moon or Mars.

Technical Outcomes

The team has finished adapting and improving a seismic imaging algorithm to ground-penetrating radar (GPR) imaging and has finished software development.
The team has also developed a dual-sparsity-based optimization algorithm to achieve super-resolution GPR imaging for noisy data. Correspondingly, the team has validated these GPR imaging techniques using various types of field data, including concrete sample, utility pipeline, tunnel, and Mars Rover GPR data.

Publications

Journal Articles

Gao, K., C. M. Donahue, B. G. Henderson and R. T. Modrak. SREMI: Super-resolution electromagnetic imaging with single-channel ground-penetrating radar. 2022. *Journal of Applied Geophysics*. **205**: 104777. (LA-UR-22-23628 DOI: 10.1016/j.jappgeo.2022.104777)

Gao, K., C. M. Donahue, B. Henderson and R. T. Modrak. SREMI: Super-Resolution Electromagnetic Imaging with Single-Channel Ground Penetrating Radar. Submitted to *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-21-32188)

Gao, K., C. M. Donahue, B. Henderson and R. T. Modrak. Deep-learning-guided high-resolution subsurface reflectivity imaging with application to ground-penetrating radar data. 2022. *Geophysical Journal International*. ggac468. (LA-UR-22-25255 DOI: 10.1093/gji/ggac468)

Presentation Slides

Albert, A. How to Detect Science BS -- Not all headlines are created equal!. . (LA-UR-23-21951)

Albert, A. How to Detect Science BS -- Not all headlines are created equal!. . (LA-UR-23-22304)

Albert, A. WIMPs are Not Dead. Presented at *P5 Town Hall at Fermilab and Argonne*, Batavia, Illinois, United States, 2023-03-21 - 2023-03-23. (LA-UR-23-22862)

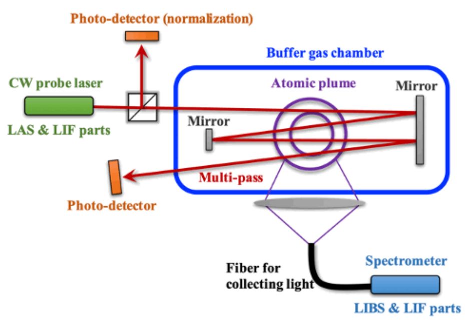
Gao, K. A Case Study and Reality Check on FWI Applied to Near-Surface Land Seismic Data. . (LA-UR-22-21412)

Gao, K., C. M. Donahue, B. Henderson and R. T. Modrak. High-fidelity GPR Image Super-resolution via Deep-supervised Machine Learning. Presented at *The International Meeting for Applied Geoscience & Energy*, Houston, Texas, United States, 2022-08-28 - 2022-09-01. (LA-UR-22-28931)

**Peer-reviewed*

Fieldable Laser Spectrometer for Elemental Analysis with Isotopic Characterization of Uranium and Plutonium

Igor Savukov
20220492MFR



The proposed laser-absorption spectroscopy (LAS)+ laser-induced breakdown spectroscopy (LIBS)+ laser-induced fluorescence (LIF) spectrometer. The continuous wave (CW) laser is the part of LAS and LIF, while the spectrometer is the part of LIBS and LIF. The normalization channel and multi-pass methods serve to improve sensitivity. The expanding atomic plume created by a pulsed laser (not shown) is depicted with two circles.

Project Description

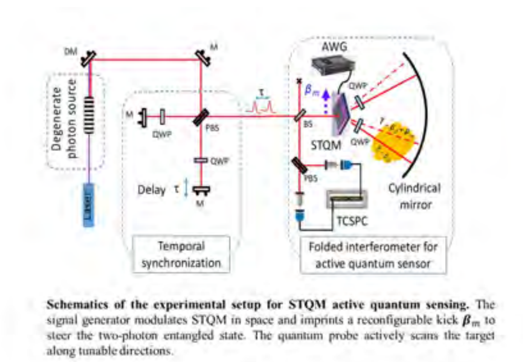
Accurate, sensitive, and fast in situ characterization of actinide isotopes (e.g. Uranium (U)-235/238) is at the core Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions. The state of the art is a bulky mass spectrometer, so the samples have to be moved to the lab and it takes a lot of time. We proposed laser spectrometer in a configuration that allows a fieldable applications for the in situ isotope characterization. First we will construct a prototype for characterization of U and plutonium (Pu) isotopes, but the method can be generalized to the characterizations of all actinides and in principles of all isotopes that have sufficiently long lifetime and sufficiently large concentration. Thus the developed instrumentation will have a great impact of the DOE/NNSA missions. Among various applications, we will initially focus on emergency response and nuclear forensics.

Technical Outcomes

The combined laser absorption spectrometer (LAS), laser induced fluorescence (LIF), and laser induced breakdown spectroscopy (LIBS) methods were tested. Experiments were conducted to improve sensitivity, using for example, laser frequency modulation, resulting in reduced background from the plasma plume. To support the development of a portable, fieldable instrument, the project tested various components: ablation laser, probe laser, and vacuum system, replacing argon buffer gas.

Dynamic Quantum Sensing

Abul Azad
20220627DI



Schematics of the experimental setup for space-time quantum metasurfaces (STQM) active quantum sensing. The signal generator modulates STQM in space and reconfigures the sensor to steer the two-photon entangled state. The quantum probe actively scans the target along tunable directions.

Project Description

Existing photonic quantum sensors lack dynamical control, hampering real time reconfiguration to rapidly scan a target of interest, and they also operate at the single frequency, limiting their abilities to sense at desired frequency bandwidth. We will address these challenges by developing novel dynamical quantum sensors based on space time quantum metasurfaces. These are compact multifunctional nanostructured electromagnetic materials that allow to harness quantum light for sensing applications. The proposed metasurface based quantum interferometers will be able to detect changes in refractive index, length, time at the utmost precision allowed by quantum mechanics, surpassing the sensitivity of any classical detection scheme. Spatiotemporal modulation offers active and dynamic functionalities to scan a target of interest both in space and in frequency. Our expected outcomes are compact multi-modal and hyper-spectral quantum sensors that go beyond the current state-of-the-art. This project will create new science and technology approaches and capabilities that contribute to the development of the National Quantum Initiative. Dynamic quantum sensors based on our groundbreaking concept of space-time quantum metasurfaces will impact Department of Energy/National Nuclear Security Administration missions on quantum sensing technologies.

Publications

Journal Articles

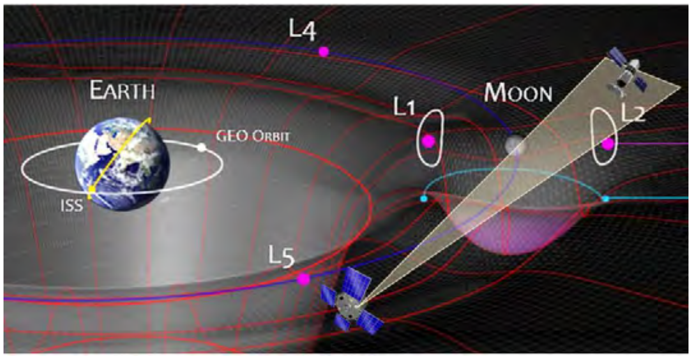
Ben-Naim, E. and P. L. Krapivsky. Statistical properties of sites visited by independent random walks. 2022. *Journal of Statistical Mechanics: Theory and Experiment*. **2022** (10): 103208. (LA-UR-22-26901 DOI: 10.1088/1742-5468/ac9619)

**Peer-reviewed*

Cislunar Space Domain Awareness

Przemyslaw Wozniak

20220798DI



The needs of Space Domain Awareness have grown beyond the radius of Geosynchronous Orbit, and now encompass the CisLunar domain. Securing this massive threat volume extending out past the Earth-Moon Lagrange point L2 presents unique challenges for multi-modal sensing networks. This project will create a framework for modeling, simulation, and analysis of sensing platforms to provide new capabilities for the robust and timely response to emerging threats in the CisLunar environment.

Project Description

Space is no longer a sanctuary, and is now a war fighting domain along with land, air and sea. This project creates new capabilities for modeling, simulation and analysis of sensing architectures necessary to secure the CisLunar environment - encompassing the Earth-Moon system. This effort is aligned with National Space Policy priorities to identify and address rapidly emerging threats in space, and perform real-time tracking of space objects for collision avoidance. Our work will have a transformational impact on Space Domain Awareness and Space Traffic Management in the CisLunar domain, and will guard against technological surprise in this new operating environment.

Publications

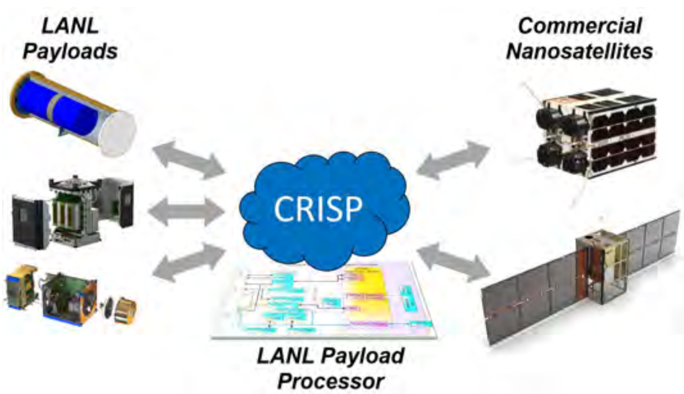
Posters

Wozniak, P. R., Y. H. Sechrest, C. R. Ward, M. W. Vance and W. Priedhorsky. Simulating Event-Driven Space Domain Awareness in Cislunar Domain. Presented at *2022 Cislunar Security Conference (CLSC)*, Laurel, Maryland, United States, 2022-11-15 - 2022-11-17. (LA-UR-22-31488)

**Peer-reviewed*

Flight Software Framework for Agile Response to Global Security Threats

Markus Hehlen
20210701DI



Integrating instrument payloads with commercial CubeSat hosts in an efficient and reliable manner is critical to an agile response to urgent and rapidly evolving global security threats. The CubeSat Reusable Interface Software Protocol (CRISP) will offer a standardized mission-agnostic software platform that is designed to transform mission agility in small satellite development and deployment.

Project Description

There is a need to deploy new space-based sensors on short timescales, for relatively low cost, and with high reliability. This level of mission agility is needed to (1) deliver actionable information on threat-relevant timescales, (2) significantly increase the cadence of developing and demonstrating new and resilient technologies in a relevant space environment, and (3) provide a framework for rapidly replenishing space assets in case of natural or manmade changes in the space environment. The two key enabling elements to create this capability are (1) leveraging commercial microsatellite technology for commodity components and services and (2) establishing a mission-agnostic technical and logistical framework that standardizes hardware, software, and workflows. The work proposed here focuses on the software component of this framework. We will develop a lean, mission-agnostic, and easy-to-maintain flight software framework that is architected and implemented specifically for microsatellite platforms. The results of this project will increase the mission agility of future microsatellite missions by streamlining the integration, testing, and operation of remote-sensing payloads. For Department of Energy/National Nuclear Security Administration, this work could enable more frequent on orbit tests and demonstrations of new sensor technology that will directly benefit the Space Nuclear Detonation Detection (SNDD) program.

Technical Outcomes

The project developed the CubeSat (a microsatellite specification standard) Reusable Interface Software Protocol (CRISP) and accompanying software as a reusable software platform enabling the rapid and reliable integration of payloads with microsatellite buses. The new code was flight-hardened and provides a framework for future missions to build upon with minimal non-recurring engineering costs. This project significantly increased the Laboratory's mission agility in the microsatellite realm and provided valuable workforce development opportunities for early-career staff members.

Publications

Conference Papers

Scobie, R. H., K. D. Kaufeld, B. J. Hoose, K. S. Morgan, K. K. Katko, M. P. Hehlen and J. M. Michel. CubeSat Reusable Interface Software Platform (CRISP): A Lightweight Message-Bus-Based Flight Software Architecture for Rapid Payload Integration. Presented at *Small Satellite Conference 2022*. (Logan, Utah, United States, 2022-08-06 - 2022-08-11). (LA-UR-22-25381)

Posters

Scobie, R. H., K. D. Kaufeld, B. J. Hoose, K. S. Morgan, K. K. Katko, M. P. Hehlen and J. M. Michel. CubeSat Reusable Interface Software Platform (CRISP): A Lightweight Message-Bus-Based Flight Software Architecture For Rapid Payload Integration. Presented at *Small Satellite Conference*, Logan, Utah, United States, 2022-08-06 - 2022-08-11. (LA-UR-22-26793)

**Peer-reviewed*

UHRGS: Ultra-High Resolution Gamma Spectroscopy for Plutonium Facility Materials Characterization

Mark Croce
20220628DI

LANL is developing a next-generation rapid and nondestructive nuclear material accounting measurement technique to improve the efficiency of operations at the nation's only Plutonium Facility. Based on ultra-high-resolution gamma spectroscopy with low-temperature microcalorimeter detectors, measurements with the prototype instrument pictured here will be used to develop the method such that it is ready for material control and accountability qualification.

Project Description

Ultra-high resolution microcalorimeter gamma spectroscopy (UHRGS) is a fundamentally new rapid, nondestructive isotopic analysis technology that provides a path to greatly reduce measurement delays in the Los Alamos National Laboratory Plutonium Facility by reducing reliance on sampling and destructive analysis. Extensive technology development over the past several years has led to the Spectrometer Optimized for Facility Integrated Applications (SOFIA) ultra-high resolution microcalorimeter gamma spectrometer being successfully deployed in a Los Alamos National Laboratory (LANL) Plutonium Facility for a fiscal year 2021 (FY21) Technology Evaluation and Demonstration (TED) project. This project will develop specific aspects of the method in order to turn it into a routine analytical capability. As a result, this work will have a wide-ranging impact on the efficiency of Plutonium Facility operations. UHRGS will provide a practical solution to characterize difficult-to-analyze materials such as plutonium 242 (242Pu) including legacy items that need to be processed or disposed of, and where sampling for destructive analysis may not be feasible.

Technical Outcomes

As the first focused research and development effort to make microcalorimeter gamma spectroscopy technology practical for Plutonium Facility (PF-4) applications in nuclear material accounting and process material characterization, this project was extremely successful as evidenced by follow-on funding received to build a dedicated instrument for PF-4. Furthermore, data from this project will continue to be used for precise determination of nuclear and atomic data needed in plutonium and americium isotopic analysis.

Publications

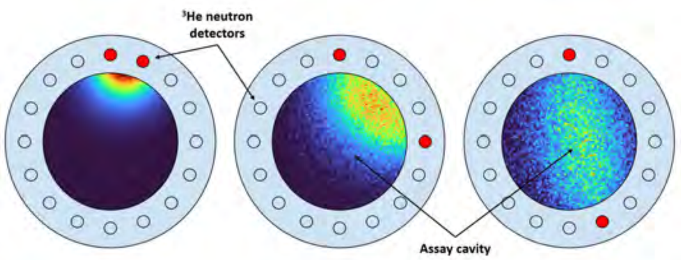
Posters

Croce, M. P., R. Winkler, E. A. Feissle, D. J. Mercer, M. H. Carpenter, K. A. Schreiber, D. G. McNeel, S. L. Weidenbenner, N. Ortiz, A. Wessels, D. Becker, J. Imrek, J. Gard, J. Mates, D. Bennett, D. Schmidt, L. Vale, D. Swetz and J. Ullom. Results from the First Deployed Ultra-High-Resolution Microcalorimeter Gamma Spectrometer. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, Kailua-Kona, Hawaii, United States, 2022-04-03 - 2022-04-03. (LA-UR-22-22784)

**Peer-reviewed*

Spatial Absorption Model for More Accurate Characterization of Transuranic Waste

Vlad Henzl
20220630DI



Transuranic waste comes in many different shapes and forms, with actual actinide sources typically being randomly distributed inside of a waste container. Their unknown position and distribution make assay with neutron coincidence counter particularly difficult and inaccurate. However, utilizing new data acquisition architecture, a.k.a. list-mode, it is possible to measure coincidences between any pair of individual helium-3 neutron detectors. As shown in the three examples above, different combination of detectors yield sensitivity to different parts of the container volume allowing effective mapping of the waste distribution.

Project Description

Transuranic (TRU) elements such as uranium and plutonium are used in many diverse missions with large part of them being of the national security importance. Be it pit production for maintenance of strategic nuclear deterrent, disassembly of excess nuclear stockpile, or fundamental actinide science, waste contaminated with, or containing, accountable amounts of TRU elements is always produced. As such, it is an unavoidable byproduct of nearly every process where TRU elements are physically handled. However, due to the physical and chemical nature of said waste - a heterogeneous mixture of diverse items, tools and materials with varying degree of TRU contamination, pseudo-randomly distributed throughout the container - the evaluation of TRU content is difficult, time consuming, and burdened with significant uncertainties that lead to substantial logistical issues and expenses. Therefore, safe and secure TRU waste disposal is a resource intensive process that may often become a bottleneck for the mission itself, leading at times to mission execution disruptions and delays. This project aims to develop new approaches – both instrumental as well as analytical – to dramatically improve TRU waste assay from the perspective of accuracy that would directly translate into streamlined, cheaper, safer, and more secure TRU waste management.

Technical Outcomes

Within the project, the Spatial Neutron Absorption model was introduced. A set of canonical source distributions in an absorptive matrix was simulated using Monte Carlo N-Particle Transport Code (MCNP) as measured by a High Level Neutron Coincidence (HLNC) Counter with list-mode data acquisition. Simulated detection rates were used to perform simple neutron tomographic imaging based on the "back-projection" technique. The project has demonstrated that with full list mode data, the source distribution can be reconstructed.

Publications

Reports

Bourque, C. M. Spatial Neutron Absorption Model: Proposal for Doctoral Dissertation Research. Unpublished report. (LA-UR-22-32891)

Presentation Slides

Bourque, C. M. MCNP: A Beginner’s Guide. . (LA-UR-22-32856)

Bourque, C. M. Spatial Neutron Absorption Model: Proposal for doctoral dissertation project. . (LA-UR-22-32859)

Bourque, C. M. and V. Henzl. Spatial Neutron Absorption Model. . (LA-UR-22-22000)

**Peer-reviewed*

Uranium Quantification in Electrodecontamination Samples via X-ray Fluorescence

John Ahern
20220635DI

Two examples of the residues from the uranium electrodecontamination (UED) process that need a rapid, in-situ means of uranium content analysis. The XRF will be used to analyze these samples and similar ones from the UED process.

Project Description

Characterization of process residues in Los Alamos National Laboratory Plutonium Facility is a required step in processing material and special nuclear material (SNM) accountability tracking. Los Alamos does not have an approved rapid in-situ method for analyzing uranium content in uranium electrodecontamination (UED) samples. Currently, the samples are removed from the glovebox line and sent to another room for analysis via methods such as calorimetry, gamma spectrometry or mass spectrometry. These methods can take days to weeks from initial generation of the residue sample to SNM content determination, depending on the length of the queue at the analytical lab. The proposed X-Ray fluorescence (XRF) spectrometers will rapidly identify and quantify uranium in-situ. This may reduce the amount of samples needing to be removed from the glovebox line and sent for more time-intensive analyses (results in minutes versus days). Characterizing more samples faster would allow for less down time waiting on measurements, therefore allow for more batches of product per year, which is vital to Los Alamos missions.

Technical Outcomes

The team collected XRF uranium data from UED samples in the plutonium facility (PF-4). They also analyzed a series of mixed plutonium/uranium Pu/U oxides from another PF-4 process and the results correlated well with the approved nuclear material control and accountability (NMCA) mass spectrometry-based measurements. The XRF method was effectively demonstrated for the mixed oxides and UED residues.

Publications

Presentation Slides

Ahern, J. C., H. E. Rasmussen, L. E. Wolfsberg, M. A. Goen, J. M. Dorhout, H. A. Quintana-Martinez, I. J. Schwerdt, G. S. Goff, S. K. Apgar and C. W. Thorn. New Process Monitoring Instruments in PF-4. Presented at *JOWOG 22-2 2022*, Aiken, South Carolina, United States, 2022-09-12 - 2022-09-16. (LA-CP-22-20658)

**Peer-reviewed*

Robust Autonomous Realtime Gas Monitoring of Safe Nuclear Waste Storage at Technical Area (TA)-55

Manvendra Dubey
20220686DI

*The project aims to deliver a tested and evaluated autonomous indoor explosive gas source location system for 24/7 monitoring and early detection of failing nuclear waste drums in indoor storage for proactive safety assurance. In figure * illustrates the gases (methane (CH4, 13CH4), ethane (C2H6), and hydrogen (H2)) venting from a failing pressurized drum that are carried by air flows in room to the sensor that then measures the gas composition with high sensitivity and speed 24/7. The trained machine learning trained inverse models finds the leaky drum using the observations of composition and air flows.*

Project Description

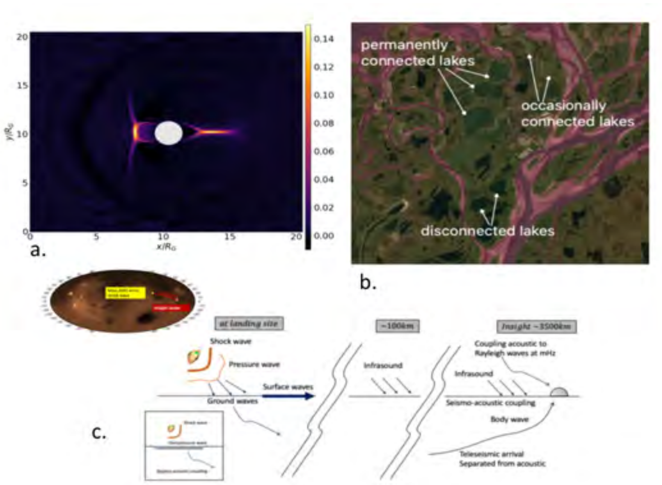
Nuclear accidents are the Achilles Heel for Weapons Production that must be managed. Currently drum inspection is done by manual off-line head-space gas analysis prior to storage. This sampling ignores the dynamic changes that occur within the drum due to changing chemistry post storage. Our clever technique enables fast autonomous detection and location of abnormal gas leakage from nuclear waste drums utilizing round the clock monitoring. No humans are involved as all the analysis and data can be analyzed by our machine learning code on the cloud and warnings issued to the operation room for prompt evaluation. The high sensitivity of our sensors allows for the detection of small gas buildup as drums pressurize upon internal heating by chemistry and should allow preemptive action prior to failure. The instruments and software are at Los Alamos and we have the expertise for indoor testing. Finally, 24/7 sampling is crucial as waste drum failures can result from transient heating at any time and will be missed by sporadic sampling of head-gas, the current control measure. Our Autonomous Low-Cost Fast Leak Detection System work for training, and then to locate sources, is transformational and will revolutionize safe nuclear waste storage.

Technical Outcomes

While the initial goals of this project were not fully realized, this work has shown the potential for non-invasive real-time reliable waste drum monitoring. Regular sniff testing of waste drums in storage can identify problematic drums earlier than current head space gas analysis. More drum sampling is needed to improve statistics and determine thresholds for action and link signals to the composition of the waste.

Center for Space and Earth Science (CSES): Foundational Research in Space and Earth Science

Lisa Danielson
20210528CR-CSE



a. Spectral Plasma Solver code density model of Ganymede that will be optimized by >10x for solution of the kinetic equations for magnetized plasmas, ultimately leading to a global magnetospheric model. b. Climate vulnerability (Colville delta, Alaska example) will be addressed by measurements of seasonal variability in delta hydrologic connectivity, to better understand how deltas alter river fluxes that drive coastal marine primary productivity. c. Entry, Descent, and Landing of Mars 2020 created different types of seismo-acoustic waves, allowing a coupling model for this uniquely known event using InSight data to accurately model impact events on the martian surface.

Project Description

This project provides national science research in the form of small, innovative, Research & Development (R&D) tasks in multidisciplinary physical sciences, along with pipelining and education opportunities that lead to filling critical roles within a wide range of national security programs within the Laboratory. The project is particularly responsive to the Department of Energy's Strategy to Advance American Space Leadership (fiscal year (FY) 2021–FY 2031), "Energy for Space." Over half the project tasks support the three strategic goals, "Solve the Mysteries of Space," "Support the Secure and Peaceful Use of Space," and "Enable the Development of Space." This project supports space exploration via technology development and fundamental research that supports our understanding of the evolution of our universe, and also addresses our ability to model, analyze, and predict outcomes of potentially hazardous natural events on the Earth's surface or within the biome, enabling our ability to enhance our national climate and biosecurity.

Publications

Journal Articles

*Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. T. Dahlin, B. Chen, G. Fleishman, L. Glesener, E. Kontar, T. Phan and C. Shen. Electron Acceleration during Macroscale Magnetic Reconnection. 2021. *Physical Review Letters*. **126** (13): 135101. (LA-UR-20-30073 DOI: 10.1103/PhysRevLett.126.135101)

Evans, A. C., A. S. Pamidi, M. B. Spano, M. H. Liu and G. A. Weiss. Immobilization and Performance of Urease in a Packed Bed Reactor 2 Evaluated with Inline Infrared Spectroscopy.. Submitted to *ACS Sustainable Chemistry & Engineering*. (LA-UR-23-22376)

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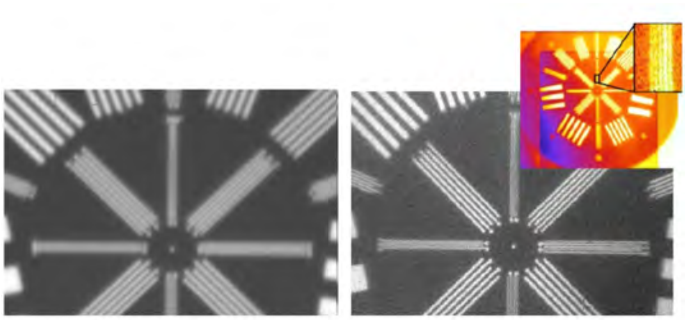
**Peer-reviewed*

Weapons Systems

Laser-Based X-ray Radiographic Imaging for Weapons Science and Applications

Brian Albright
20220018DR



Maximal extractable value (MeV) radiography of a test object from a Microtron beam source (left) and a laser-based x-ray source (right), showing the improved resolution and image clarity possible with a laser-based MeV x-ray source, with its much smaller x-ray spot size (< 100 micrometers). Developing this proof-of-principle technology demonstration into a deployable technology for weapons science and other applications is the goal of this project. If successful, this will enable the deployment of flexible, inexpensive, compact x-ray sources for static tomographic radiography and dynamic multi-axis radiography at our firing sites and facilities such as pRad and U1a.

Project Description

We seek to develop novel x-ray sources based on high-power short-pulse lasers with unique advantages including small spot size, flexible configuration, and tailorable spectra. This will allow Los Alamos National Laboratory to deploy flexible, compact x-ray sources for static tomographic radiography and dynamic multi-axis radiography at our firing sites (where we perform high-explosive-driven dynamic experiments) and other important National Nuclear Security Administration facilities such as Protron Radiography (pRad) Complex and U1a Complex. The higher resolution, shorter pulse duration, and tunability of our sources will enable new applications in the weapons program and broader scientific community. This effort applies unique Los Alamos National Laboratory expertise and capability in high-power laser-plasma interaction science, radiography, numerical modeling, and target fabrication.

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Luedtke, S. V., A. Favalli, C. Huang, M. J. Schmitt, A. G. Seaton, A. Sood, D. J. Stark, L. Yin, J. E. Coleman, D. C. Gautier, C. E. Hamilton, J. F. Hunter, B. J. Jones, M. L. Klasky, A. J. Mendez, S. Palaniyappan, J. R. Strehlow, C. D. Tomkins and B. J. Albright. Developing Predictive Modeling of Laser-Plasma Interactions for X-ray Radiographic Imaging. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30543)

Luedtke, S. V., A. Favalli, C. Huang, M. J. Schmitt, A. G. Seaton, A. Sood, D. J. Stark, L. Yin, S. A. Bruce, J. E. Coleman, T. Ditmire, D. C. Gautier, C. E. Hamilton, J. F. Hunter, B. J. Jones, M. L. Klasky, E. Medina, A. J. Mendez, S. Palaniyappan, H. J. Quevedo, M. M. Spinks, J. R. Strehlow, C. D. Tomkins and B. J. Albright. Developing Predictive Modeling of Laser-Plasma Interactions for X-ray Radiographic Imaging. Presented at *Annual Anomalous Absorption Conference*, Skytop, Pennsylvania, United States, 2022-06-06 - 2022-06-10. (LA-UR-22-25222)

Luedtke, S. V., N. P. Tan, R. F. (. Bird, S. L. Harrel, M. Taufer and B. J. Albright. VPIC 2.0: Performance-Portable Particle-in-Cell for Present and Future Supercomputers. Presented at *International Conference on Numerical Simulation of Plasmas (ICNSP)*, Online, Japan, 2022-08-30 - 2022-09-02. (LA-UR-22-28924)

Palaniyappan, S. Laser-Driven MeV X--Ray Radiography. Presented at *LaserNetUS*, Fort Collins, Colorado, United States, 2022-08-18 - 2022-08-18. (LA-UR-22-28776)

Palaniyappan, S., D. C. Gautier, J. R. Strehlow, B. J. Albright, L. Yin and J. F. Hunter. MeVXRay-23A: We aim to increase the laser-driven MeV x-ray yield to ~ 4-6 Rads/shot (~2-3\xef \xbc\xb8 increase) using novel target designs suitable for weapons radiography. . (LA-UR-22-22451)

Stark, D. J., C. Huang, S. V. Luedtke, M. J. Schmitt, A. G. Seaton, L. Yin, F. N. Beg, A. Bogale, S. A. Bruce, G. Capeluto, H. Chen, E. A. Chowdhury, J. E. Coleman, T. Ditmire, J. C. Fernandez, R. Fitzgarrald, D. C. Gautier, C. E. Hamilton, R. Hollinger, J. F. Hunter, B. J. Jones, M. L. Klasky, E. Medina, A. J. Mendez, L. M. T. Mix, S. Palaniyappan, H. J. Quevedo, J. J. Rocca, A. Sood, M. M. Spinks, J. R. Strehlow, A. G. R. Thomas, C. D. Tomkins, J. Twardowski, A. K. Van Pelt and B. J. Albright. Developing Predictive Modeling of Laser-Plasma Interactions for X-ray Radiographic Imaging. Presented at *LaserNetUS User*, Fort Collins, Colorado, United States, 2022-08-16 - 2022-08-18. (LA-UR-22-28545)

Posters

Albright, B. J., S. Palaniyappan, L. Yin, A. S. Bogale, J. F. Hunter, J. E. Coleman, J. C. Fernandez, R. J. Fitzgarrald, D. C. Gautier, C. E. Hamilton, C. Huang, B. J. Jones, M. L. Klasky, S. V. Luedtke, L. M. T. Mix, M. J. Schmitt, A. Sood, D. J. Stark, J. R. Strehlow, C. D. Tomkins, J. D. Twardowski and A. K. Van Pelt. Development of laser-based MeV photon sources for static and dynamic radiography. Presented at *64th Meeting of the American Physical Society Division of Plasma Physics*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30531)

Albright, B. J., S. Palaniyappan, L. Yin, J. F. Hunter, A. Bogale, J. E. Coleman, J. C. Fernandez, R. J. Fitzgarrald, D. C. Gautier, C. E. Hamilton, C. Huang, B. J. Jones, M. L. Klasky, L. M. T. Mix, M. J. Schmitt, A. Sood, D. J. Stark, J. R. Strehlow, C. D. Tomkins, J. D. Twardowski, A. K. Van Pelt and S. V. Luedtke. (U) Development of laser-based MeV photon sources for static and dynamic radiography. Presented at *Nuclear Explosives Design Physics Conference (NEDPC)*, Livermore, California, United States, 2022-11-07 - 2022-11-11. (LA-CP-22-20782)

Huang, C., B. J. Albright, A. S. Bogale, J. E. Coleman, A. Favalli, J. C. Fernandez, R. J. Fitzgarrald, D. C. Gautier, C. E. Hamilton, J. F. Hunter, B. J. Jones, M. L. Klasky, S. V. Luedtke, A. J. Mendez, S. Palaniyappan, M. J. Schmitt, A. G. Seaton, A. Sood, D. J. Stark, J. R. Strehlow, C. D. Tomkins, J. D. Twardowski and L. Yin. Simulation of laser preplasma interaction with ionization dynamics. Presented at *64th Annual Meeting of the APS Division of Plasma Physics*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30648)

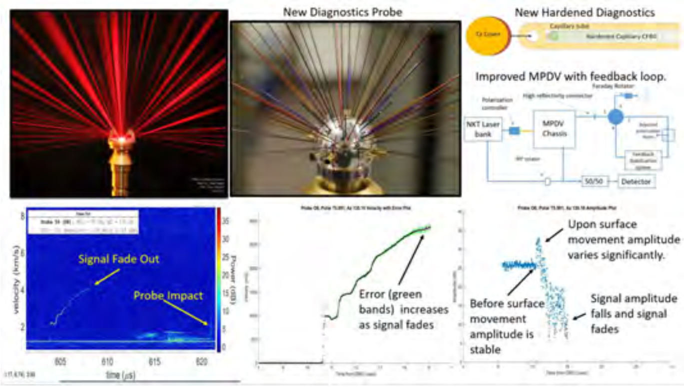
Strehlow, J. R., F. N. Beg, A. Bogale, S. A. Bruce, G. Capeluto, H. Chen, J. E. Coleman, T. Ditmire, J. C. Fernandez, R. Fitzgarrald, D. C. Gautier, C. Huang, C. E. Hamilton, R. Hollinger, J. F. Hunter, B. J. Jones, M. L. Klasky, S. V. Luedtke, E. Medina, J. A. Mendez, L. M. T. Mix, S. Palaniyappan, H. Quevedo, J. J. Rocca, M. J. Schmitt, A. G. Seaton, A. Sood, M. M. Spinks, D. J. Stark, A. G. R. Thomas, C. D. Tomkins, J. Twardowski, A. K. Van Pelt, L. Yin, B. J. Albright and E. A. Chowdhury. Laser-driven MeV x-ray sources for radiography. Presented at *Joseph Strehlow*, Fort Collins, Colorado, United States, 2022-08-16 - 2022-08-16. (LA-UR-22-28388)

Strehlow, J. R., F. N. Beg, A. S. Bogale, S. A. Bruce, G. Capeluto, H. Chen, E. Chowdhury, J. E. Coleman, T. Ditmire, J. C. Fernandez, R. Fitzgarrald, D. C. Gautier, C. Huang, C. E. Hamilton, R. Hollinger, J. F. Hunter, B. J. Jones, M. L. Klasky, S. V. Luedtke, E. Medina, A. J. Mendez, L. M. T. Mix, S. Palaniyappan, H. Quevedo, J. Rocca, M. J. Schmitt, A. G. Seaton, A. Sood, M. Spinks, D. J. Stark, A. Thomas, C. D. Tomkins, J. Twardowski, A. K. Van Pelt, L. Yin and B. J. Albright. Laser-driven MeV x-ray sources for radiography. Presented at *Annual Meeting of the American Physical Society (APS) - Division of Plasma Physics (DPP)*, Spokane, Washington, United States, 2022-10-17 - 2022-10-21. (LA-UR-22-30708)

**Peer-reviewed*

Determining the Causes of Multiplexed Photonic Doppler Velocimetry (MPDV) Signal Loss During a Dynamic Experiment

Daniel Kalb
20220025DR



Multiplex Photonic Doppler Velocimetry (MPDV) measures the velocity of a moving surface with laser beams (upper left). The raw data is processed into the spectrogram (lower left) and shows signal fade out. The velocity profile (lower center) is extracted from the spectrogram and error increases as signal fades. The amplitude of the velocity signal (lower right) varies once surface movement begins and drops significantly. Improved and new new diagnostics (upper right and center) will be tested. This project investigates the causes of early signal drop out and will propose solutions.

Project Description

Managing the nuclear stockpile requires hydrodynamic testing and modeling. Since the moratorium on underground testing (1992), the nation has relied on hydrodynamic experiments (hydrotests) using surrogate materials and advance diagnostics to validate our models and certify the stockpile. As the stockpile ages, hydrotests become more crucial than ever. The current state of the art diagnostics are radiography and Multiplexed Photonic Doppler Velocimetry (MPDV). MPDV uses laser interferometry, measuring implosion characteristics, velocity over time. These data are critical for proving the adequacy of the models used to simulate nuclear weapons performance. This indispensable diagnostic has suffered from early signal drop out, resulting in data sets that are not as complete as desired, missing late time data. The causes of the early signal dropout are not fully known or understood, but many factors have been identified and need to be investigated. This project will use experiments and modeling to determine which factors are significant, propose and test solutions, develop alternate diagnostics, and improve the process to develop experimental requirements for future hydrotests. Using the findings from this project, the final deliverable will be a design guide, laying out the steps to design and field a successful hydrotest for future experimenters and designers.

Publications

Presentation Slides

Birge, N. W., K. T. Hughes and P. Younk. Method to dynamically measure the optical return loss from shocked metal surfaces. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-10 - 2022-07-16. (LA-UR-22-26545)

Birge, N. W., K. T. Hughes and P. Younk. (U) Method to dynamically measure the optical return loss from shocked metal surfaces. . (LA-CP-22-20886)

Birge, N. W., V. Geppert-Kleinrath, C. R. Danly, V. E. Fatherley, M. S. Freeman, H. J. Jorgenson, E. F. Mendoza, L. R. Tafoya, C. H. Wilde, P. Younk, K. T. Hughes and D. Fittinghoff. Extending neutron imaging capabilities for Inertial Confinement Fusion. . (LA-UR-22-25848)

Hughes, K. T., N. W. Birge and P. Younk. Performance of momentum diagnostics when impinged with a high-speed jet of explosive products. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, White Rock, New Mexico, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26454)

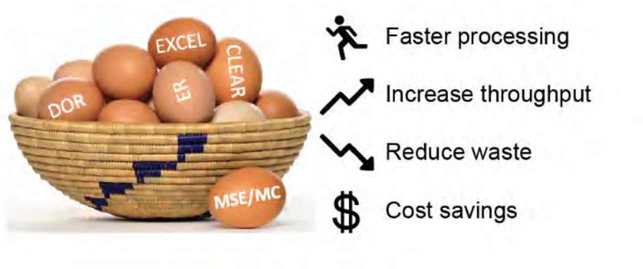
Hughes, K. T., N. W. Birge and P. Younk. (U) Small-scale experiments to study the performance of PDV when subjected to a high-velocity jet. Presented at *NEDPC 2022*, White Rock, New Mexico, United States, 2022-11-07 - 2022-11-10. (LA-CP-22-20771)

Sullivan, G. K., P. Younk and P. I. Miller. Kickoff Meeting for Determining the Causes of Multiplexed Photonic Doppler Velocimetry (MPDV) Signal Loss During a Dynamic Experiment. Presented at *LDRD Kickoff Meeting for DR Project 20220025DR.*, Los Alamos, New Mexico, United States, 2021-10-27 - 2021-10-27. (LA-UR-21-30424)

**Peer-reviewed*

Diversifying Large-Scale Plutonium (Pu) and Americium (Am) Processing

Stosh Kozimor
20220054DR



Pit production at LANL has a single point failure associated with Pu and Am processing. All the eggs are in one basket. This project will diversify Pu and 241Am processing at the Molten Salt Extraction (MSE) step and help to build an agile capability for manufacturing weapons systems.

Project Description

Disposing of plutonium (Pu) and americium (Am) pyrochemical waste costs Los Alamos National Laboratory $10M/year. Costs would be higher without Pu/Am reprocessing efforts in the Los Alamos Actinide Material Processing & Power and Pit Technology divisions, which save ~$15M/year. The 30 pits per year mission is estimated to increase these waste disposal and processing costs substantially ($48M/year by FY26). Management recognizes this problem and the need for fundamental research that advances processing efforts. This proposal addresses that need and outlines a research and development campaign to diversify and strengthen Pu and Am processing capabilities.

Publications

Journal Articles

Arko, B. T., D. Dan, S. L. Adelman, D. B. Kimball, S. A. Kozimor, J. C. Shafer and B. Stein. Electron Transfer Between Neptunium and Sodium Chlorite in Acidic Chloride Media. Submitted to *Inorganic Chemistry*. (LA-UR-23-22229)

Arko, B. T., D. Dan, S. L. Adelman, D. B. Kimball, S. A. Kozimor, M. M. Martinez, T. Mastren, D. L. Huber, V. Mocko, J. H. Rim, J. C. Shafer, B. Stein and E. M. I. Wylie. Exploring how exposure to radiolysis and harsh chemical reagents impact americium-241 extraction chromatography. 2022. *Materials Advances*. (LA-UR-22-27095 DOI: 10.1039/D2MA00859A)

*DiMucci, I. M., H. D. Root, Z. R. Jones, S. A. Kozimor, M. M. MacInnes, J. L. Miller, V. Mocko, W. J. Oldham and B. W. Stein. Photochemical separation of plutonium from uranium. 2022. *Chemical Communications*. **58** (78): 10961-10964. (LA-UR-22-25083 DOI: 10.1039/D2CC04225H)

Gilhula, J. C., L. Xu, F. D. J. White, S. L. Adelman, K. E. Aldrich, E. R. Batista, D. Dan, Z. R. Jones, S. A. Kozimor, R. L. Meyer, N. Thiele, P. Yang and M. Yuan. Overcoming Challenges Facing the Complexation of Weakly Electrophilic Metal Cations, Like Ra2+, Ba2+, and Sr2+. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-23-22661)

Li, B., Z. R. Jones, C. Eiroa Lledo, K. E. Knope, V. Mocko, B. Stein, J. N. Wacker, S. A. Kozimor, E. R. Batista and P. Yang. Structure and Dynamics of NaCl/KCl/CaCl2-EuCln (n=2, 3) Molten Salts. Submitted to *Inorganic Chemistry*. (LA-UR-22-32935)

Rice, N. T., E. Danielou Dalodiere, S. L. Adelman, Z. R. Jones, S. A. Kozimor, V. Mocko, H. D. Root and B. Stein. OXIDIZING AMERICIUM(III) WITH SODIUM BISMUTHATE IN ACIDIC AQUEOUS SOLUTIONS. Submitted to *Inorganic Chemistry*. (LA-UR-22-21284)

Stein, B., M. Y. Livshits, S. A. Kozimor, N. J. Wolford, S. M. Greer, J. K. Banh, K. Hanson, M. MacInnes and J. S. R. Vellore Winfred. Exploring Differences in Lanthanides Excited State Reactivity Using a Simple Example: The Photophysics of La and Ce Thenoyltrifluoroacetone (TTA) Complexes. Submitted to *Inorganic Chemistry*. (LA-UR-22-32634)

Reports

Arko, B. T. Advances in Americium-241 Processing. Unpublished report. (LA-UR-23-23148)

Arko, B. T., S. L. Adelman, D. B. Kimball and S. A. Kozimor. Selective Precipitations 2 Invention Disclosure. Unpublished report. (LA-UR-23-22931)

Pereiro, F. A. and S. S. Galley. Manipulation of ligand electronic structure to control f-element covalency. Unpublished report. (LA-UR-23-23499)

Presentation Slides

Arko, B. T. CHARACTERIZING EXTRACTION CHROMATOGRAPHY FOR LARGE-SCALE AMERICIUM-241 PROCESSING. Presented at *Actinide Separations Conference*, Los Alamos, New Mexico, United States, 2022-05-17 - 2022-05-17. (LA-UR-22-24332)

Arko, B. T. Advances in Large-Scale 241Am Production. . (LA-UR-23-22937)

DiMucci, I. M. REVEALING UNCONVENTIONAL ELECTRONIC STRUCTURE USING MULTI-EDGE X-RAY ABSORPTION SPECTROSCOPY. . (LA-UR-21-32192)

Piedmonte, I. D. Shining a Light on Plutonium Separations. . (LA-UR-22-31668)

Posters

Li, B., E. R. Batista and P. Yang. Multi-scale Modeling of Nuclear Energy Materials. Presented at *Kavli Frontiers of Science 19th Chinese American Symposium*, Irvine, California, United States, 2022-07-08 - 2022-07-10. (LA-UR-22-26617)

Sharma, S., B. Li, P. Yang and E. R. Batista. Effect of Outer-Coordination Sphere on Redox Potential of Lanthanide and Actinide Chlorides in Molten Salts. Presented at *2nd International Workshop on Theory Frontiers in Actinide Science : Chemistry & Materials*, Santa Fe, New Mexico, United States, 2023-02-26 - 2023-03-01. (LA-UR-23-21752)

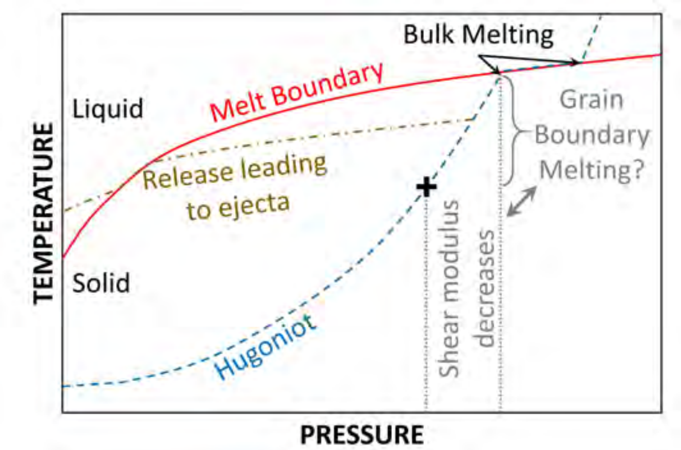
Other

Li, B., E. R. Batista and P. Yang. Dataset of Understanding the Structural, Dynamical, Chemical and Thermophysical Properties of Molten Chlorides for Molten Salt Reactors using Electronic Structure Methods. Dataset. (LA-UR-23-20714)

**Peer-reviewed*

Examining the Influence of Liquid Localized at Grain Boundaries on Dynamic Wave Propagation

Matthew Beason
20220679DR



In typical metals the elastic shear modulus begins decreasing (black plus) at 70-80% of the shock pressure where bulk melting is observed along the Hugoniot (blue). The behavior along the Hugoniot serves as a starting point for materials response under dynamic loading. Whether grain boundary melting occurs or not will have a dramatic impact on models predicting ejecta, strength, and recompression. This project will determine whether grain boundary melting explains the observed reduction in shear modulus by examining the behavior of the Aluminum-Gallium (Al+Ga) system, where it can be shown that a locallized liquid phase forms exclusively along grain boundaries.

Project Description

Shock melting occurs when a material is impacted at sufficiently high velocities that it is compressed to the point of melting. How shock melting relates to the equilibrium equation of state (relationship between pressure, volume, and temperature) has long been in dispute. Measurements of the elastic properties observed at increasing shock pressures shows a reduction in elastic shear modulus. It has been suggested that this indicates localized melting along grain boundaries; however, bulk melting has been observed to occur at higher shock pressures. Limits in measurement resolution have complicated efforts to determine whether a liquid phase is forming along the grain boundaries. This project seeks to determine whether a trace liquid phase leads to the reduction in shear modulus prior to bulk melting. Instead trying to prove whether a liquid phase forms along grain boundaries under shock loading, we will introduce a liquid phase along the grain boundaries of artificial intelligence (AI) and observe its influence on the dynamic wave propagation and elastic shear modulus. Where a liquid phase occurs under dynamic loading is pivotal to developing multiphase equations of state (the backbone of hydrocode simulations) and physics based modeling of strength and ejecta formation.

Technical Outcomes

The project team was able to produce an aluminum gallium composite material to examine whether liquid forming along grain boundaries leads to a reduction in shear modulus. The team was also able to develop a method allowing pyrometry to examine the melt boundary of aluminum gallium at millibar pressures. This is a significant achievement that will impact ongoing work in the field.

Publications

Presentation Slides

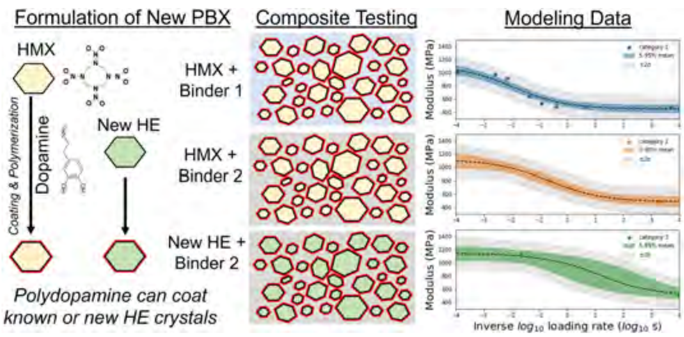
Beason, M. T., T. M. Hartsfield and B. J. Jensen. Dynamic Measurements of the Al Melt Boundary. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-26628)

Beason, M. T. and B. J. Jensen. Examining the Transition Enthalpy of Sn from Shock Melting. Presented at *American Physical Society (APS) March Meeting*, Las Vegas, Nevada, United States, 2023-03-06 - 2023-03-10. (LA-UR-23-22206)

**Peer-reviewed*

Biologically Inspired Coatings for Advanced Plastic-bonded Explosive (PBX) Formulations

Nathan Miller
20220138ER



Many thermal and mechanical properties of plastic-bonded explosives (PBX) are affected or even dominated by the structure and properties of the crystal-polymer interface. Nonfavorable interactions between a desired high explosive (HE) and a binder can even prevent successful formulation. Using polydopamine or other adhesion promoters, we can both tailor the properties of the formulated composites and enable new formulations to be manufactured. Using hierarchical Bayesian inference we can incorporate data from disparate systems to model behavior of this class of materials. This enables simulations, with quantified uncertainties, of the anticipated response of novel materials with limited additional experimental evidence.

Project Description

Currently, creating fully qualified new explosive materials is time consuming and expensive, while developing necessary models to describe the explosive behavior requires a large number of tests. To address this challenge, the high level goals of this project are to make substantial advances in timeline, cost and versatility of explosive manufacturing and the corresponding engineering model development. Both of these are critical for meeting Los Alamos National Laboratory and national goals for greatly improved throughput of new materials development for next generation weapons systems. We expect that these advanced explosives will offer future engineers and scientists great flexibility in designing novel experiments, weapons and technologies. We could also use this manufacturing innovation to customize properties of current stockpile explosives. The engineering models developed in this project will greatly increase our understanding of fundamental behavior in these materials. If successful, the number of experiments needed to predict material behavior will be massively reduced, saving time and money. In summary, if everything works, by the end of the project we should have the technology to create an effectively unlimited number of new explosive materials and be able to predict many explosive properties using only a very small number of fundamental observations and tests.

Publications

*Peer-reviewed

Journal Articles

Herman, M. J., C. Liu, E. B. Watkins, N. A. Miller, A. L. Duque and J. D. Yeager. Biologically inspired reinforcement using polydopamine of polymer bound composites. 2023. *Composites Part B: Engineering*. 110563. (LA-UR-22-25031 DOI: 10.1016/j.compositesb.2023.110563)

Herman, M. J., E. B. Watkins and J. D. Yeager. Structural Properties, and Qualities of Aqueous Grown Polydopamine Thin Films Determined by Neutron Reflectometery. Submitted to *ACS Applied Materials & Interfaces, or Macromoecules*. (LA-UR-22-27773)

Reports

Herman, M. J. Advance Formulation of Highly Loaded Composites via Biomimetic Interfacial Reinforcement. Unpublished report. (LA-UR-22-29939)

Presentation Slides

Herman, M. J. Advanced Formulation of Highly Loaded Composites via Biomimetic Interfacial Reinforcement. . (LA-UR-22-29703)

Herman, M. J., A. L. Duque, C. Liu, N. A. Miller and J. D. Yeager. Formulation Advancements via Biologically Inspired Core-Shell Coating Technique for Plastic Bonded Explosives and High-Fidelity Mocks. Presented at *JANNAF 2021*, Online, NM, New Mexico, United States, 2021-12-06 - 2021-12-16. (LA-UR-21-31634)

Herman, M. J., C. Liu, A. L. Duque, L. G. Hill and J. D. Yeager. Mechanical and Explosive Performance Modifications of PBXs via Biologically Inspired Core-shell Surface Coating. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-11 - 2022-07-15. (LA-UR-22-25732)

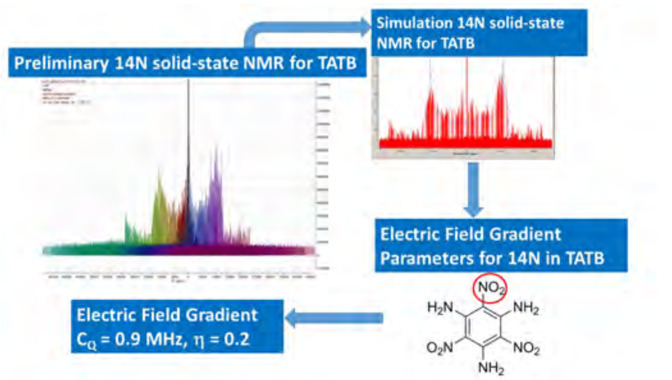
Herman, M. J., C. Liu, E. B. Watkins, N. A. Miller, A. L. Duque and J. D. Yeager. Interfacial Investigation of High Loaded Plastic Bonded Explosive Interfaces Modified via Biologically Inspired Core-Shell Coating Technique. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-28 - 2022-03-03. (LA-UR-22-21689)

Herman, M. J., J. D. Yeager and E. B. Watkins. Film Structure of Polymerized Synthetic Dopamine by Neutron Reflectometry. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, San Diego, California, United States, 2023-03-20 - 2023-03-24. (LA-UR-23-21870)

Miller, N. A. (U) Estimation of lot-dependent explosive material properties using hierarchical Bayesian inference. Presented at *JOWOG 31 HOCWOG*, Aldermaston, United Kingdom, 2022-06-27 - 2022-06-30. (LA-CP-22-20387)

Identifying Structure-Property Relationships in High Explosives: Using Nitrogen-14 Nuclear Magnetic Resonance (NMR) to Determine Processing Differences and Defect Effects in Materials

Michael Janicke
20210876ER



Determining the electric field gradient parameters is a step-wise process and a key metric to determine structure-performance relationships. This will be achieved by complementary nitrogen-14 (14N) NMR measurements, Density functional theory (DFT) calculations, and the systemic study of many TATB (2,4,6-triamino-1,3,5- trinitrobenzene) systems. Shown here is initial results for the NO2 for TATB. 14N NMR results (left), simulation (upper right), electric field gradient (EFG) predictions (lower left).

Project Description

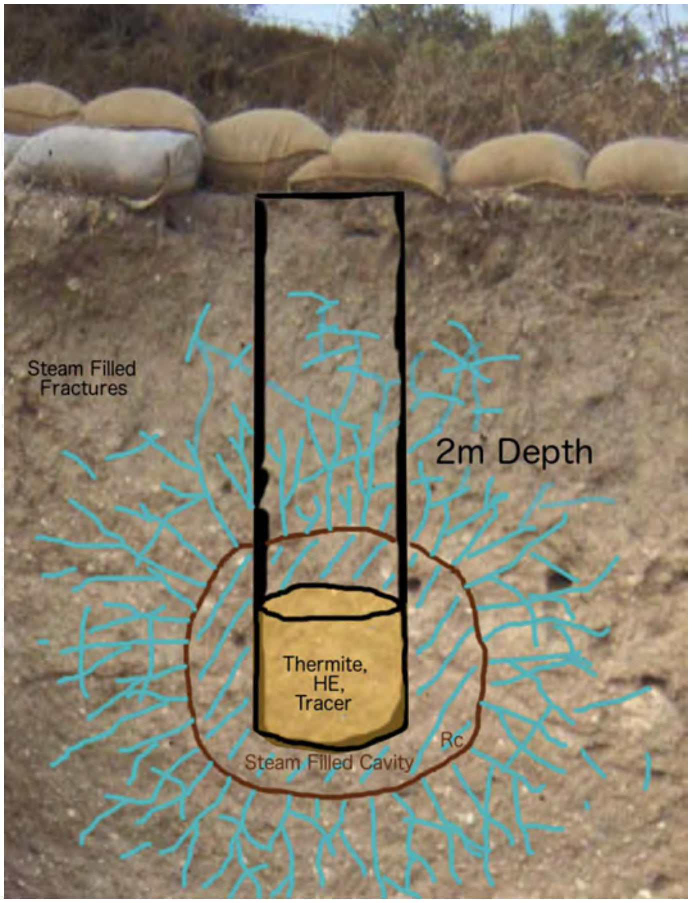
“What is a detonation wave in this microscopic approach and which are the problems to be analyzed in order to define the molecular and crystalline conditions which characterize a molecular crystal as an explosive? In other words, more directly, in order to bring some answer to the question: 'why does an explosive explode' or if you prefer why could it not explode?” This quote taken from a computational paper titled “Fundamental Physics and Chemistry Behind Molecular Crystal Detonations at a Microscopic Level” eloquently outlines many of the challenges facing Los Alamos National Laboratory's (LANL’s) chemistry approaches in the field of energetic materials. Detailed knowledge of the atomic and microstructure of nitrogen based mission-relevant materials (i.e. explosives) is fundamental to our understanding them: as they age, as we re-engineer them to replace materials in the stockpile, as they become part of ever evolving accident and threat scenarios. This team is utilizing existing LANL technology and expertise to demonstrate that Nuclear Magnetic Resonance (NMR), the foundation of Magnetic Resonance Imagine (MRI), can safely, quantitatively, and non-destructively characterize materials of high mission relevance and address some of these issues raised above.

Technical Outcomes

The results from this project have helped to push the Nuclear Magnetic Resonance work at Los Alamos forward by identifying the hardware deficiencies that need to be resolved.

Advancing Containment Science in Unconsolidated Environments

Garrett Euler
20220667ER



High-quality data of non-isothermal, multi-component, multiphase flow & transport of explosive byproducts in the shallow subsurface are lacking. The LDRD team will conduct a helium experiment at the LANL firing site Minie this spring using modern containment diagnostics to assess cutting-edge, multi-disciplinary simulation capabilities.

Project Description

We will collect scientific data on the subsurface flow & transport of gases and debris using an underground conventional explosion, test diagnostic instruments, and advance cutting-edge simulation packages to improve Los Alamos National Laboratory containment science. This set of generated capabilities could impact our nation's ability to safely conduct underground experiments in new environments and to monitor for unannounced low-yield nuclear experiments based on advances in our understanding of coupling to ground motion and the mobility of near-surface explosive byproducts.

Technical Outcomes

This project successfully developed and executed a containment experiment in a shallow, poorly consolidated setting at Los Alamos with newly developed diagnostics that measured key containment phenomena that will provide constraints on geologic material models and simulations of explosive cavity formation and subsurface tracer gas migration. These provide advances in Los Alamos' ability to contain low yield experiments in these challenging geologic environments and allow additional flexibility in the planning of future weapons programs.

Publications

Other

Meijer, W. Z. and G. G. Euler. Containment Pipe Drawings & SOLIDWORKS Files. Dataset. (LA-UR-22-26820)

**Peer-reviewed*

A Modeling and Experimental Approach to Optimizing the Explosive Source for Blast-Tube Tests

Philip Rae
20220680ER

A test explosion in the LANL Blast Tube Facility showing the slight products venting at the tube sections. The aim of this project is to distribute the explosion over the whole length of the tube rather than as a single monolithic explosive charge as used in this particular test.

Project Description

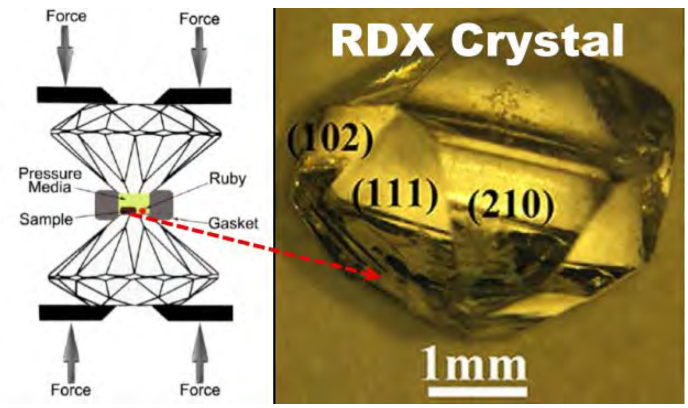
Blast environment testing of nuclear weapon reentry bodies and vehicles is of ongoing interest. This project aims to improve the unique capability Los Alamos National Laboratory currently has so that defined pressure pulse shapes and magnitudes may be estimated accurately using computer modeling and transitioned to real world tests with fewer tests. Additionally, we aim to reduce the damage potential from our current mode of operation so that testing becomes faster and cheaper. We aim to move away from using a conventional military grade explosive owing to the violence it imparts to the blast tube facility and instead use a gentler composition mixed at Los Alamos. By tailoring the explosive it is planned that much of the fireball currently emitted from the end of the tube after detonation can be eliminated making the soft catch pit designed to slow the test article simpler to design.

Technical Outcomes

The team designed, built, commissioned and tested a new mini blast tube to prove out a new concept that may be used in future for the large blast tube facility at Lower Slobbovia. Three tests were undertaken and pressure data captured. These data compare favorably with computer modeling predictions. Suggested improvements for the mini blast tube facility have been identified that would improve the data fidelity and improve the functionality of the site.

An Exploration of the Phase Diagrams and Piezoelectric Properties of High Explosive Crystals at Extreme Conditions

Bethany Hopp
20210943PRD2



The image shows a schematic of a Diamond Anvil Cell (DAC) on the left, and the explosive crystal RDX. The DAC is the main experimental thrust of this work and will be used to reach high pressure states in order to map out the RDX phase diagram. RDX is used in the vast majority of military explosive applications. The ability to predict the behavior of this material is extremely important in terms of the nation's security interests. This work seeks to explore the currently unexplored electrical nature of some of the phases reached in the shock initiation of RDX.

Project Description

This work intends to study the phase diagram of the explosive crystal cyclotrimethylenetrinitramine (RDX) with an emphasis on the piezoelectric properties of each phase. RDX is an explosive crystal commonplace in conventional and nuclear weapons, both in the United States stockpile, but also utilized by foreign nations not aligned to US interests. The accurate modeling of explosives is important in both the design and disablement of such weapons. It is imperative that all phenomenon encountered in the detonation of such devices are included in such modeling. To date no effort has included the occurrence of piezoelectricity in phases on the detonation pathway. In this project the piezoelectric nature of the RDX will be explored with the aim to provide experimental data that will underpin Los Alamos National Laboratory's modelling efforts in this field.

Publications

Presentation Slides

Chidester, B. A., M. Harwell, J. Badro, D. Spaulding, M. Huff, P. Kalita, R. Caracas, S. B. Jacobsen and S. Stewart. Shock response of a magma ocean analog to 1 TPa. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31967)

Chidester, B. A., M. Millot, J. Badro, R. Caracas, E. Davies, D. Fratanduono, M. L. Harwell, M. Huff, S. B. Jacobsen, P. Kalita, S. Root, D. Spaulding, J. Townsend and S. Stewart. Experimental temperature measurements of Fe-bearing silicate minerals and glasses to 1.6 TPa. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-06 - 2022-07-15. (LA-UR-22-26404)

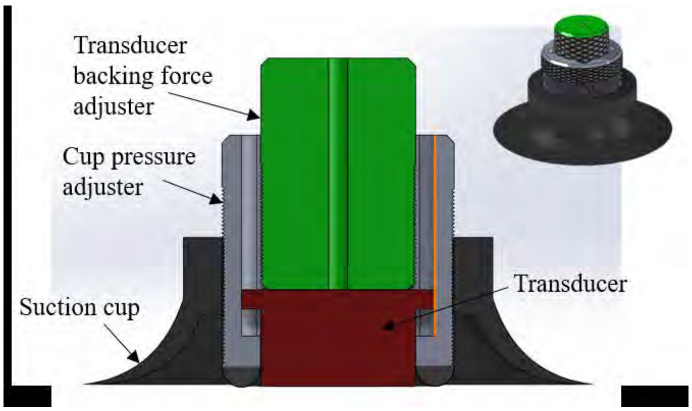
Posters

Chidester, B. A., M. J. Burns, M. J. Cawkwell, B. Sturtevant and D. M. Dattelbaum. High-pressure, high-temperature phase diagram and equations of state of RDX polymorphs. Presented at *American Physical Society (APS) Shock Compression of Condensed Matter*, Anaheim, California, United States, 2022-07-06 - 2022-07-15. (LA-UR-22-26417)

**Peer-reviewed*

Design of Sensor System for Repeatable Acoustic Resonance Measurements

John Greenhall
20220495MFR



Concept for an Acoustic Resonance Spectroscopy transducer system that enables repeatable attachment of the transducer to an object under inspection.

Project Description

The ability to rapidly and noninvasively identify internal structural changes such as damage, corrosion, or pressure changes within a system are of great interest to the Surveillance, Weapons Production, and Emergency Response communities. Acoustic measurements are highly sensitive to such internal changes, but they are also sensitive to the orientation and backing force that is used to hold the acoustic transducers on the object. Thus, we are developing a transducer system to enable repeatable transducer orientation and backing force to ensure that changes in the acoustic measurements are due to the structural changes in the object. Additionally, we are developing a methodology to simplify the acoustic measurements, which consist of a large number of overlapping peaks. This simplified representation will then lead to improved damage/pressure measurement accuracy through machine learning techniques.

Publications

Journal Articles

Greenhall, J. J., P. K. Kendall, A. L. Graham, D. N. Sinha and C. Pantea. Genetic algorithm-wavelet transform feature extraction for acoustic resonance spectroscopy machine learning or regression. Submitted to *IEEE Transactions on Signal Processing*. (LA-UR-22-23887)

Presentation Slides

Greenhall, J. J., E. S. Davis, P. K. Kendall, A. L. Graham, D. N. Sinha and C. Pantea. Extracting useful machine learning features from acoustic resonance spectra of coupled multi-body structures. Presented at *Acoustical Society of America (ASA) - Spring Meeting*, Denver, Colorado, United States, 2022-05-23 - 2022-05-27. (LA-UR-22-23492)

Greenhall, J. J., E. S. Davis, P. Vakhlamov, C. A. Chavez, A. L. Graham, D. N. Sinha and C. Pantea. Noninvasive Pressure Measurements Using Acoustic Resonance Spectroscopy (ARS). Presented at *IEEE International Ultrasonics Symposium*, venice, Italy, 2022-10-10 - 2022-10-14. (LA-UR-22-29304)

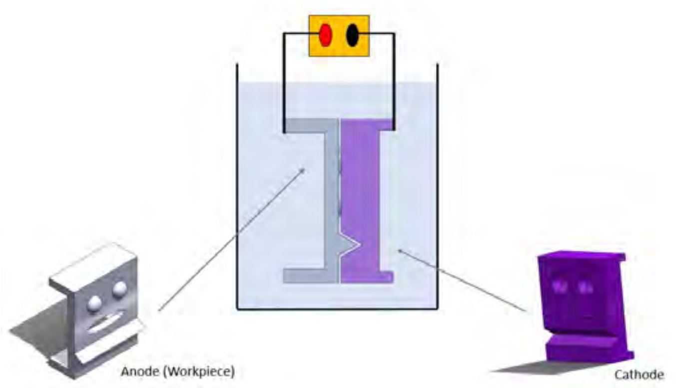
Posters

Greenhall, J. J., E. S. Davis, P. Vakhlamov, C. A. Chavez, A. L. Graham, D. N. Sinha and C. Pantea. Noninvasive Pressure Measurements Using Acoustic Resonance Spectroscopy. Presented at *IEEE International Ultrasonics Symposium*, Venice, Italy, 2022-10-10 - 2022-10-14. (LA-UR-22-29027)

**Peer-reviewed*

Optimizing Metal Surface Finish Through Advanced Manufacturing Processes

Courtney Clark
20220504MFR



While electropolishing is considered a standard electrochemical surface finishing process, utilization of metal additively manufactured (MAM) conforming electrodes is a novel concept. LANL is working to develop and optimize the use of MAM conforming electrodes, as well as fixturing apparatus for a range of standard electrochemical processes.

Project Description

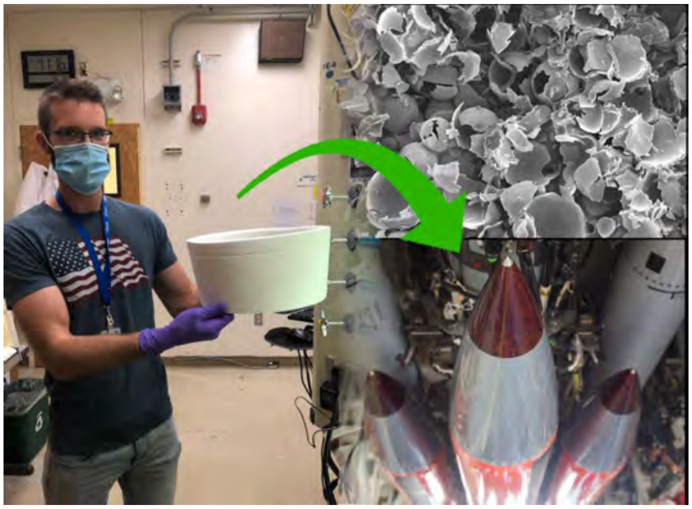
There is urgent need to develop advanced manufacturing techniques to create a more agile manufacturing workflow. Electrochemical surface finishing processes, including electropolishing, electroplating, and anodizing are commonly employed for improving the surface quality of many components. Integration of metal additively manufactured (MAM) fixtures and conforming electrodes into these electrochemical finishing processes will present reduction opportunities for design-build-certification costs and work timelines for Los Alamos National Laboratory, National Nuclear Security Administration partners, and the broader commercial industry. Not only can advanced manufacturing, and metal additive manufacturing, be used as stand-alone techniques, they can also be utilized as support for conventional manufacturing processes, furthering modernization of advanced manufacturing technology as a whole. The ultimate motivation of this project is to establish advanced manufacturing, specifically MAM, processes as a baseline for full-scale developments in industry, putting the Laboratory at the forefront of innovation. Successful proof of concept will open up a very large commercial space for this fundamentally new technology, allowing fully-customizable MAM fixtures for surface finishing to be integrated into routine industrial practice.

Technical Outcomes

The project goal was to improve rough metal additively manufactured surfaces to meet engineering requirements while maintaining their geometrical fidelity. Multi-angle test geometries and conforming counter electrodes for electropolishing were printed from low carbon (316L) stainless steel using laser beam-powder bed fusion. A 10 times improvement in roughness was obtained for the optimized parameters, with minimal geometry deformation. A simplified model was developed that allowed a tailored counter electrode geometry to shape the developing current density profile.

Enabling Design Agility in a Joint Test Assembly Flight Body

John Minotti
20210962DI



The image depicts the development of a more agile process in the design, model, build, test sequence for FTBs (flight test bodies). Through novel laboratory synthesis and characterization techniques recently pioneered at LANL, new candidate materials for flight testing applications may be more quickly and thoroughly screened and evaluated for their most vital properties and behaviors. As an example, a novel structural mount prototype is shown (left) along with its micro-structure (top right).

Project Description

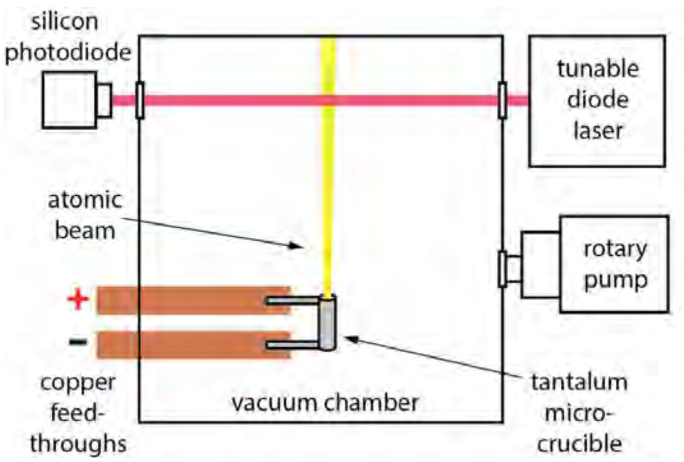
New materials with enhanced properties and behaviors are continually being developed for use in weapons systems. However, there is currently a large disconnect between the fabrication of a new material component and the ability to rapidly assess its benefits in a real-world environment. This is not only due to a lack of collegial research-based interactions between materials scientists with weapons systems engineers, but also from a long, arduous process of specifying requirements and ensuring that any new material meets or exceeds these in their entirety. Put simply, these obstacles have resulted in many new and potentially useful materials sitting "on the shelf" with no clear path to serving the nation in any meaningful way. This project seeks to modernize the manner in which new materials are screened, tested and optimized in flight environments. Here the team will utilize new technologies for polymer cushions and structural mounts as an illustrative example of how process flexibility in materials synthesis techniques can aid in developing a more agile and responsive methodology for evaluating these materials in real-world environments. This work is a collaboration between materials science researchers and the Flight Integration Engineering group at Los Alamos National Laboratory.

Technical Outcomes

To streamline weapon system development, the team iteratively developed component requirements with material science and component processing experts' input. Processing methodologies and characterization parameters of a novel syntactic foam were mapped to component needs to tailor strength, density, and thermal conductivity specifications. The goal to optimize the design, build, test, and iterate feedback loop was only partially received due to staff turnover.

Portable Isotopic Analyzer in Support of Plutonium Manufacturing

Alonso Castro
20220649DI



Schematic diagram of the method for rapid isotopic analysis of plutonium in an atomic beam. A resistively-heated micro-crucible generates an atomic beam that is interrogated by a tunable diode laser. The resulting spectrum reveals the isotopic composition of the sample.

Project Description

This project will allow the rapid isotopic analysis of plutonium samples at the point of generation, without the need for sample preparation or chemical separation steps, and without the need for complex and expensive mass spectrometric analysis. This ability for rapid isotopic analysis will enable drastic reductions in turn-around time throughout the weapons manufacturing process flowsheet by eliminating bottle-necks created by the time-consuming nature of mass spectrometry. The proposed system has the potential to greatly enhance the Laboratory mission agility in the area of plutonium manufacturing.

Technical Outcomes

This project was successful in achieving the proposed goals. The team set up an atomic beam laser spectroscopy system for isotopic analysis of plutonium in the Chemistry and Metallurgy Research building. An isotopic spectrum of plutonium at 421 nanometers with excellent signal-to-noise ratio was obtained. The isotopic composition of a Certified Reference Material was obtained from the spectral isotopic data.

LABORATORY DIRECTED
RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

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