Los Alamos National Laboratory

Laboratory Directed Research and Development

FY20 Annual Progress Report: Compendium of Project Summaries

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Los Alamos NATIONAL LABORATORY

LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

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, and Science of Signatures. Project summaries for continuing projects appear first, followed by project summaries and technical outcomes for projects that ended in FY20.

Los Alamos LDRD project identification numbers consists of three parts. The first is the fiscal year in which the project was initially funded, the second is a unique numerical identifier, and the third identifies the project component.

Publications identified throughout the project summaries that are marked with an "*" are confirmed to be peer reviewed publications.

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Project Summaries: Table of Contents

Complex Natural and Engineered Systems

Information Science and Technology

Materials for the Future

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Science of Signatures

Complex Natural and Engineered Systems

Understanding Actinide-Water Interactions in High Pressure-Temperature (P-T) Environments

Hongwu Xu
20180007DR

Project Description

The overarching goal of this project is to transform our understanding on the speciation, solubility and stability of actinide-bearing phases in high-pressure high-temperature aqueous environments using an integrated experimental and modeling approach. This new field of actinide science has important relevance to a range of nuclear applications and is tied to DOE/NNSA missions in energy and national security. More specifically, successful execution of this project will contribute greatly to addressing the needs to develop accident-tolerant nuclear fuels, build the safety basis for permanent disposal of the tens of thousands of metric tons of spent nuclear fuel accumulated at power plants, and understand actinide environmental signatures from underground nuclear testing in support of Global Security applications. In addition, this project will afford a new unique capability of wide-ranging utility to the DOE complex in the fields of actinide science and technology, as well as materials and chemical systems beyond actinides.

Publications

Journal Articles

Akram, N., D. Dhakal, R. A. Mayanovic, H. Boukhalfa and H. Xu. A Study of Uranyl (VI) Chloride Complexes in Aqueous Solutions under Hydrothermal Conditions using Raman Spectroscopy. Submitted to *MRS Advances*. (LA-UR-20-22166)

Baker, J. L., G. Wang, T. Ulrich, J. T. White, E. R. Batista, P. Yang, R. C. Roback, C. Park and H. Xu. High-pressure structural behavior and elastic properties of U3Si5: A combined synchrotron XRD and DFT study. 2020. *Journal of Nuclear Materials*. **540**: 152373. (LA-UR-20-22625 DOI: 10.1016/j.jnucmat.2020.152373)

*Chung, C., E. C. O'Quinn, J. C. Neuefeind, A. F. Fuentes, H. Xu, M. Lang and A. Navrotsky. Thermodynamic and structural evolution of mechanically milled and swift heavy ion irradiated Er2Ti2O7 pyrochlore. 2019. *Acta Materialia*. **181**: 309-317. (LA-UR-19-24244 DOI: 10.1016/j.actamat.2019.09.022)

*Chung, C., M. Lang, H. Xu and A. Navrotsky. Thermodynamics of radiation induced amorphization and thermal annealing of Dy 2 Sn 2 O 7 pyrochlore. 2018. *Acta Materialia*. **155**: 386-392. (LA-UR-18-22912 DOI: 10.1016/j.actamat.2018.06.003)

*Chung, C., X. Guo, G. Wang, T. L. Wilson, J. T. White, A. T. Nelson, A. Shelyug, H. Boukhalfa, P. Yang, E. R. Batista, A. A. Migdisov, R. C. Roback, A. Navrotsky and H. Xu. Enthalpies of formation and phase stability relations of USi, U3Si5 and U3Si2. 2019. *Journal of Nuclear Materials*. **523**: 101-110. (LA-UR-19-21352 DOI: 10.1016/j.jnucmat.2019.05.052)

*Dhakal, D., R. A. Mayanovic, J. L. Baker, H. Boukhalfa, H. Xu and C. Sun. Design of a containment apparatus for synchrotron XAS measurements of radioactive fluid samples under high temperatures and pressures. 2019. *Review of Scientific Instruments*. **90** (8): 083108. (LA-UR-19-23291 DOI: 10.1063/1.5100887)

Gabitov, R., A. Migdissov, A. Nguyen, N. F. van Hartesveldt, A. Perez-Huerta, A. Sadekov, K. B. Sauer, J. L. Baker, V. Paul, F. A. Caporuscio, H. Xu and R. C. Roback. Uptake of uranium by carbonate crystallization from reduced and oxidized hydrothermal fluids. 2021. *Chemical Geology*. **564**: 120054. (LA-UR-20-28097 DOI: 10.1016/j.chemgeo.2020.120054)

Goncharov, V., N. Wei, M. L. Lau, S. M. Ennaceur, A. Migliori, H. Xu, M. Long and X. Guo. Thermodynamic and elastic properties of cerium doped yttrium aluminum garnets. Submitted to *Chemistry of Materials*. (LA-UR-20-24352)

*Guo, X., J. T. White, A. T. Nelson, A. Migdisov, R. Roback and H. Xu. Enthalpy of formation of U3Si2 : A high-temperature drop calorimetry study. 2018. *Journal of Nuclear Materials*. **507**: 44-49. (LA-UR-18-22051 DOI: 10.1016/j.jnucmat.2018.04.032)

*Guo, X., X. Lu, J. T. White, C. J. Benmore, A. T. Nelson, R. C. Roback and H. Xu. Bulk moduli and high pressure crystal structure of U3Si2. 2019. *Journal of Nuclear Materials*. **523**: 135-142. (LA-UR-19-22091 DOI: 10.1016/j.jnucmat.2019.06.006)

*Kalintsev, A., A. Migdisov, H. Xu, R. Roback and J. Brugger. Uranyl speciation in sulfate-bearing hydrothermal solutions up to 250\xe2\x80\xaf\xc2\xb0C. 2019. *Geochimica et Cosmochimica Acta*. **267**: 75-91. (LA-UR-19-20322 DOI: 10.1016/j.gca.2019.08.027)

Kalintsev, A., A. Migdissov, C. D. Alcorn, J. L. Baker, J. Brugger, R. Mayanovic, N. Akram, H. Xu, H. Boukhalfa, F. A. Caporuscio, H. S. Viswanathan, C. Jove-Colon, Y. Wang, E. Matteo and R. C. Roback. Loss of a Titan: Uranium carbonate complexes at elevated temperatures. Submitted to *Nature Geoscience*. (LA-UR-20-30270)

Lee, S., H. Xu and H. Xu. Reexamination of the structure of opal-A: A combined study of synchrotron X-ray diffraction and pair distribution function analysis. Submitted to *American Mineralogist*. (LA-UR-20-23036)

*Liu, M., Q. Kang and H. Xu. Modelling uranium dioxide corrosion under repository conditions: A pore-scale study of the chemical and thermal processes. 2020. *Corrosion Science*. **167**: 108530. (LA-UR-19-28033 DOI: 10.1016/j.corsci.2020.108530)

Liu, M., Q. Kang and H. Xu. Grain-scale Study of the Grain Boundary Effect on UO2 Fuel Oxidation and Fission Gas Release Under Reactor Condition. Submitted to *Chemical Engineering Journal*. (LA-UR-20-21237)

Liu, M., Q. Kang and H. Xu. Three-Dimensional Physics-Based Modelling of Nuclear Fuel Dissolution at Grain Scale. Submitted to *Corrosion Science*. (LA-UR-20-26401)

*Liu, M., V. Starchenko, L. Anovitz and A. Stack. Grain detachment and transport clogging during mineral dissolution in carbonate rocks with permeable grain boundaries. 2020. *Geochimica et Cosmochimica Acta*. **280**: 202-220. (LA-UR-19-23804 DOI: 10.1016/j.gca.2020.04.022)

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*Migdisov, A., X. Guo, H. Nisbet, H. Xu and A. E. Williams-Jones. Fractionation of REE, U, and Th in natural ore-forming hydrothermal systems: Thermodynamic modeling. 2019. *The Journal of Chemical Thermodynamics*. **128**: 305-319. (LA-UR-18-27417 DOI: 10.1016/j.jct.2018.08.032)

Migdissov, A., H. D. Nisbet, N. Li, J. T. White, H. Xu, A. Nelson and R. C. Roback. Instability of U3Si2 in pressurized water media at elevated temperatures. Submitted to *Nature Communications*. (LA-UR-20-27557)

Migdissov, A., N. F. van Hartesveldt, A. Kalintsev, H. D. Nisbet, C. D. Alcorn, A. C. Strzelecki, R. Ram, H. Boukhalfa, H. Xu, R. Gabitov, J. Brugger, B. Etschmann, C. Jove-Colon, E. Matteo, F. A. Caporuscio, R. C. Roback and J. T. White. An unexplored uranium mobilization pathway from nuclear waste repositories. Submitted to *Nature Energy*. (LA-UR-19-30310)

Nisbet, H. D., A. Migdissov, A. E. Williams-Jones, V. van Hinsberg, H. Xu and R. C. Roback. The solubility of thorium in carbonate-bearing solutions at hydrothermal conditions. Submitted to *Geochimica et Cosmochimica Acta*. (LA-UR-20-30269)

Nisbet, H. D., A. Migdissov, A. Williams-Jones, H. Xu, V. van Hinsberg and R. C. Roback. Challenging the Th-immobility paradigm: The high stability of Th-SO42- complexes at elevated temperature. Submitted to *Science*. (LA-UR-19-20286)

*Nisbet, H., A. Migdisov, H. Xu, X. Guo, V. van Hinsberg, A. E. Williams-Jones, H. Boukhalfa and R. Roback. An experimental study of the solubility and speciation of thorium in chloride-bearing aqueous solutions at temperatures up to 250\xe2\x80\xaf\xc2\xb0C. 2018. *Geochimica et Cosmochimica Acta*. **239**: 363-373. (LA-UR-18-22200 DOI: 10.1016/j.gca.2018.08.001)

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Wang, G., E. R. Batista and P. Yang. Water on actinide dioxide surfaces: a review of recent progresses. Submitted to *Crystals*. (LA-UR-20-24006)

Wang, G., P. Yang and E. R. Batista. Computational screening of 2D coatings for semiconducting photocathodes. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-29869)

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Xu, H., X. Guo, D. Wu, S. V. Ushakov, T. Shvareva and A. Navrotsky. Energetics of hydration on uranium oxide and peroxide surfaces. Submitted to *Journal of Materials Research*. (LA-UR-19-22695)

*Xu, H., X. L\xc3\xbc, P. J. Heaney and Y. Ren. Structural behavior of a stuffed derivative of \xce\xb1-quartz, Mg0.5AlSiO4, at

high temperature: an in situ synchrotron XRD study. 2019. *Physics and Chemistry of Minerals*. **46** (7): 717-725. (LA-UR-19-21198 DOI: 10.1007/s00269-019-01033-1)

Books/Chapters

Migdissov, A., H. Xu, A. E. Williams-Jones and J. Brugger. The REEs in Hydrothermal Systems. (LA-UR-18-23654)

Presentation Slides

Baker, J. L. High-Pressure Structural Behavior and Bulk Modulus of U3Si5. Presented at *2019 COMPRES Annual Meeting*, Big Sky, Montana, United States, 2019-08-02 - 2019-08-05. (LA-UR-19-27174)

Baker, J. L. Material Properties at Extreme Pressures and Temperatures. . (LA-UR-20-26623)

Baker, J. L., D. Dhakal, N. Akram, R. Mayanovic, X. Guo, T. L. Ulrich, J. T. White, A. Migdissov, G. Wang, C. Sun, E. R. Batista, P. Yang, A. Chen, H. Boukhalfa, R. C. Roback, C. Park, A. J. Gaunt and H. Xu. Structure and Properties of Uranium-Bearing Solid and Aqueous Phases at High P/T Conditions. . (LA-UR-20-26398)

Baker, J. L., D. Dhakal, R. Mayanovic, X. Guo, A. Migdissov, C. Sun, S. Heald, E. R. Batista, P. Yang, H. Boukhalfa, A. J. Gaunt and H. Xu. Understanding Actinide-Water Interactions in High P-T Environments Using X-Ray Absorption Spectroscopy. Presented at *LDRD Project Appraisal Review*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20556)

Baker, J. L., J. T. White, A. Chen, R. C. Roback and H. Xu. Specific Heat Measurements on USi from 2.4K to 398K. Presented at *MRS Fall Conference*, Boston, Massachusetts, United States, 2019-12-01 - 2019-12-05. (LA-UR-19-31767)

Boukhalfa, H., J. L. Baker, H. Xu, N. Li, D. Dhakal, R. Mayanovic and C. Chung. Materials synthesis & characterization. . (LA-UR-19-20644)

Chung, C., A. Navrotsky, H. Xu and M. K. Lang. Thermodynamics and Stabilities of Radiation Damaged Pyrochlore Ceramic Nuclear Waste Forms and U Si Based Fuel Compounds. . (LA-UR-19-26405)

Chung, C., X. Guo, J. T. White, A. Nelson, A. Shelyug, H. Boukhalfa, R. C. Roback, A. Navrotsky and H. Xu. Energetics of Uranium Silicides. Presented at *Goldschmidt 2018*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-12. (LA-UR-18-27575)

Guo, X., H. Xu, C. Armstrong, C. Parker, K. Kriegsman, K. Popa, H. Boukhalfa, J. N. Mitchell, M. Ramos, A. J. Gaunt and R. C. Roback. High-temperaturedrop-solutioncalorimetryofPuO2: preliminarystudies. Presented at *2019 ACS National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-03-31. (LA-UR-19-22849)

Guo, X., H. Xu, H. Boukhalfa, R. C. Roback, J. N. Mitchell, J. T. White, A. T. Nelson, A. J. Gaunt and C. Armstrong. Experimental thermodynamics and solid-state chemistry on actinide-containing materials. Presented at *ACS NORM*, Richland, Washington, United States, 2018-06-24 - 2018-06-24. (LA-UR-18-25408)

Guo, X., X. L\xc3\xbc, J. T. White, A. Nelson, C. Benmore, R. C. Roback and H. Xu. Bulk Moduli and High-Pressure Crystal Structures of Uranium Silicides. Presented at *MS&T 2018*, Columbus, Ohio, United States, 2018-10-15 - 2018-10-15. (LA-UR-18-30051)

van Hartesveldt, N. F., A. Migdissov, R. C. Roback, H. Xu and R. Gabitov. Stability of U(IV) sulfate complexes at elevated temperatures. Presented at *Goldschmidt*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27631)

Kalintsev, A., A. Migdissov, H. Xu, R. C. Roback and J. Brugger. Complexation behaviour of uranyl in sulfate-bearing solutions at elevated temperatures. Presented at *Goldschmidt 2018*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27632)

Kang, Q. Pore-Scale Reactive Transport Modeling. . (LA-UR-19-20671)

Kang, Q., Y. Chen and A. J. Valocchi. Final Report of Institutional Computing Project w19_porescale: Figures. . (LA-UR-20-21775)

Kelley, M. P., X. Zhang, J. Su, P. Yang, E. R. Batista, J. L. Baker, A. Migdissov, H. Boukhalfa and H. Xu. AnO2-Cl Coordination Chemistry at High P/T. . (LA-UR-19-20639)

Liu, M. Reactive transport in porous media: A pore-scale perspective. . (LA-UR-19-28552)

Liu, M., Q. Kang and H. Xu. Direct Numerical Simulations of Coupled Physicochemical and Thermal Processes Involved in Actinide-Fluid Interactions. Presented at *Goldschmidt 2020*, Honolulu, Hawaii, United States, 2020-06-21 - 2020-06-26. (LA-UR-20-24291)

Mayanovic, R., D. Dhakal, H. Xu and H. Boukhalfa. In-Situ Raman Spectroscopy of Actinide Species and Compound. Presented at *LDRD DR Project Appraisal Meeting*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20542)

Migdissov, A., H. Xu and H. Boukhalfa. The Peculiar Behavior of U and Th in Hydrothermal Solutions. . (LA-UR-18-25393)

Migdissov, A., H. Xu and H. Boukhalfa. Complexation of U and Th in Hydrothermal Solutions. Presented at *Migration 2019*, Kyoto, Japan, 2019-09-15 - 2019-09-20. (LA-UR-19-29119)

Migdissov, A., N. F. van Hartesveldt, A. Kalintsev, H. D. Nisbet, H. Xu, F. A. Caporuscio, H. Boukhalfa, R. C. Roback and J. Brugger. Re-visiting Hydrothermal Speciation of Uranium. Presented at *Goldschmidt 2019*, Barcelona, Spain, 2019-08-18 - 2019-08-23. (LA-UR-19-28187)

Migdissov, A., X. Guo, H. D. Nisbet, N. F. van Hartesveldt, A. Kalintsev, H. Xu, H. Boukhalfa, R. C. Roback, V. van Hinsberg, A. E. Williams-Jones, R. I. Gabitov and J. Brugger.

Geochemical controls of mobilisation, deposition, and fractionation of REE, U, and Th in ore forming hydrothermal systems. Presented at *Goldschmidt 2018*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-18. (LA-UR-18-27542)

Nisbet, H. D., A. Migdissov, H. Xu, A. Williams-Jones, V. van Hinsberg, X. Guo, H. Boukhalfa and R. C. Roback. The solubility and speciation of thorium in chloride-bearing aqueous solutions at elevated temperatures. Presented at *Goldschmidt Conference 2018*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-18. (LA-UR-18-27541)

Nisbet, H. D., A. Migdissov, R. C. Roback, H. Xu, A. E. Williams-Jones and V. van Hinsberg. The Behavior of Thorium in REE-Bearing Hydrothermal Fluids. Presented at *Goldschmidt Conference*, Barcelona, Spain, 2019-08-18 - 2019-08-23. (LA-UR-19-27954)

White, J. T., A. P. Shivprasad, C. J. Grote, J. T. Dunwoody, D. D. Byler, C. Chung, S. S. Parker, N. Wozniak and H. Xu. Synthesis & Fabrication of Uranium and Thorium Nuclear Fuels. Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20714)

White, J. T., S. Widgeon Paisner, D. M. Frazer, T. L. Ulrich, B. P. Nolen, J. R. Wermer, C. J. Grote, J. T. Dunwoody, D. D. Byler and H. Xu. Synthesis & Fabrication of Nuclear Fuel Materials. Presented at *LDRD-DR review*, Los Alamos, New Mexico, United States, 2020-02-13 - 2020-02-13. (LA-UR-20-21407)

Xu, H. Structural Behavior, Thermal Expansion & Phase Relations of \xce\xb2-Eucryptite at Variable-T & High-P Conditions. Presented at *MS&T19*, Portland, Oregon, United States, 2019-09-30 - 2019-09-30. (LA-UR-19-29897)

Xu, H. Thermochemistry of Materials for Sustainable Nuclear Energy. . (LA-UR-19-32497)

Xu, H., A. J. Gaunt, A. Migdissov, J. T. White, H. Boukhalfa, E. R. Batista, P. Yang, Q. Kang, S. A. Kozimor, F. A. Caporuscio, J. N. Mitchell, J. L. Baker, H. D. Nisbet, C. Chung, M. P. Kelley, G. Wang, N. F. van Hartesveldt, A. Kalintsev, A. S. Ditter, D. Dhakal, R. Mayanovic, J. Brugger, A. Navrotsky and S. Heald. Understanding Actinide-Water Interactions in High P-T Environments. Presented at *LDRD DR Project Appraisal Meeting*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20624)

Xu, H., A. Migdissov, A. Timofeev, H. D. Nisbet, A. Kalintsev, N. F. van Hartesveldt, R. Gabitov, F. A. Caporuscio, J. Brugger, J. T. White, A. Nelson, H. Boukhalfa, E. R. Batista and P. Yang. Understanding Actinide-Water Interactions in High P-T Environments. Tasks 2 (Spectroscopy, UV-Vis) and 3 (Solubility): Determination of thermodynamic properties of aqueous species and solid phases at high T and P. . (LA-UR-19-20555)

Xu, H., A. Migdissov, H. Boukhalfa and R. C. Roback. Speciation and Stability of Uranium and Thorium in Hydrothermal Environments. Presented at *MS&T2019*, Portland, Oregon, United States, 2019-09-29 - 2019-09-29. (LA-UR-19-29408)

Xu, H., R. Mayanovic, D. Dhakal, J. L. Baker, X. Guo, M. P. Kelley, P. Yang, E. R. Batista, C. Sun, H. Boukhalfa, A. Migdissov and R. C. Roback. Uranyl-Chloride Speciation at Hydrothermal Conditions. Presented at *Goldschmidt2019*, Barcelona, Spain, 2019-08-18 - 2019-08-18. (LA-UR-19-27925)

Xu, H., X. Guo, C. Chung, A. Migdissov, J. T. White, A. T. Nelson and R. C. Roback. Thermodynamic Stability of Uranium Silicides. Presented at *The 22nd meeting of the International Mineralogical Association*, Melbourne, Australia, 2018-08-12 - 2018-08-12. (LA-UR-18-27545)

Xu, H., X. Guo, C. Chung, A. Migdissov, J. T. White, N. Li, A. Nelson, R. C. Roback and A. Navrotsky. Structure and Stability of Uranium Silicides for Nuclear Fuel Applications. Presented at *2019 ACS National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-03-31. (LA-UR-19-22746)

Xu, H., X. Guo, C. Chung, J. T. White, J. N. Mitchell, H. Boukhalfa, A. J. Gaunt, A. Migdissov, G. Wang, P. Yang, E. R. Batista and A. Navrotsky. Calorimetric Studies of Actinide Compounds. Presented at *LDRD DR Project Appraisal Meeting*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20543)

Posters

Baker, J. L., J. T. White, R. C. Roback, C. Park and H. Xu. High-Pressure Structural Behavior and Bulk Modulus of U3Si5. Presented at *2019 COMPRES Annual Meeting*, Big Sky, Montana, United States, 2019-08-02 - 2019-08-05. (LA-UR-19-27177)

Chung, C., X. Guo, J. T. White, A. T. Nelson, A. Shelyug, H. Boukhalfa, R. C. Roback, A. Navrotsky and H. Xu. Enthalpies of Formation and Phase Stabilities of U-Si Materials. Presented at *ThermoCon Workshop 2018*, Pullman, Washington, United States, 2018-07-23 - 2018-07-23. (LA-UR-18-26568)

Kalintsev, A., A. Migdissov, H. Xu, R. C. Roback and J. Brugger. U(VI) speciation in hydrothermal carbonate-bearing fluids up to 250 \xc2\xbaC. Presented at *Migration 2019*, Kyoto, Japan, 2019-09-15 - 2019-09-20. (LA-UR-20-21350)

Liu, M., Q. Kang and H. Xu. Modelling of Uranium Dioxide Corrosion under Flow Conditions. Presented at *AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31438)

Migdissov, A. Hydrothermal Studies of Actinides at LANL (EES-14): Predictive Capabilities for Repositories, Nuclear Reactors, Environmental, and Non-Proliferation Science. . (LA-UR-18-21516)

Nisbet, H. D., A. Migdissov, H. Xu, X. Guo, V. van Hinsberg, A. Williams-Jones, H. Boukhalfa and R. C. Roback. An experimental investigation into the behavior of thorium in aqueous solution at elevated temperature. Presented at *LANL Student Symposium 2018*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-26874)

Xu, H., A. Migdissov, H. D. Nisbet, A. Kalintsev, N. F. van Hartesveldt, J. L. Baker, H. Boukhalfa, R. C. Roback, R. Mayanovic, D. Dhakal and N. Akram. Speciation, Stability and Mobility of Uranium and Thorium in Hydrothermal Environments. Presented at *GSA Annual Meeting*, Phoenix, Arizona, United States, 2019-09-22 - 2019-09-22. (LA-UR-19-29065)

Other

Yang, P., X. Zhang, M. P. Kelley, J. Su and E. R. Batista. Dataset of Density Functional Theory simulations of molecular systems. Dataset. (LA-UR-18-31843)

Adaptation Science for Complex Natural-Engineered Systems

Donatella Pasqualini
20180033DR

Project Description

Half of U.S. population and gross domestic product (GDP) is located in coastal counties. Electrical, water, and other critical infrastructure necessary to support population centers and the nation's economic and national security is disproportionally concentrated on the coast. Coastal regions are at risk of extreme flooding due to major storms, such as Hurricanes Katrina and Sandy, combined with the erosion of shorelines and stress on wetlands which protect the coast, and these risks may increase. This project will address two challenges: (1) predicting how coastlines will change over the next few decades due to the combined action of storms, waves, erosion, groundwater pumping, and other factors; and (2) designing electrical-water infrastructure networks in coastal regions that are more resilient to the flood and saltwater damage anticipated to occur in a changed coastal zone. We will develop a new coastal model that simulates and predicts the complex evolution of the coastline due to ocean, vegetation, and land surface interactions; and an optimization model that redesigns large infrastructure networks for resilience to natural hazards. The result will improve U.S. energy and national security and economic prosperity, by protecting the nation's electrical grid and other infrastructure assets upon which communities and industry depend.?

Publications

Journal Articles

Brus, S. R., P. J. J. Wolfram and L. Van Roekel. Unstructured global to coastal wave modeling for the Energy Exascale Earth System Model. Submitted to *Geoscientific Model Development*. (LA-UR-20-27828)

Cao, Z., P. J. J. Wolfram, C. Friedrichs, J. C. Rowland and Y. Zhang. A Data-driven Approach to Predict Sediment Settling Velocity. Submitted to *Joint Special Issue on Coastal Hydrology and Oceanography for Water Resources Research and Journal of Geophysical Research: Oceans*. (LA-UR-19-25788)

Cao, Z., P. J. J. Wolfram, J. C. Rowland, Y. Zhang and D. Pasqualini. Estimating Sediment Settling Velocities from a Theoretically Guided Data-Driven Approach. 2020. *Journal of Hydraulic Engineering*. **146** (10): 4020067. (LA-UR-20-22942 DOI: 10.1061/(ASCE)HY.1943-7900.0001798)

Cao, Z., Y. Zhang, P. J. J. Wolfram, S. R. Brus, J. C. Rowland, C. B. Begeman, C. Xu and D. Pasqualini. Analysis of vegetation drag parameterizations for coastal hydrodynamic modeling. Submitted to *Environmental Modelling & Software*. (LA-UR-21-20703)

Francom, D. C. and B. Sanso. BASS: An R Package for Fitting and Performing Sensitivity Analysis of Bayesian Adaptive Spline Surfaces. Submitted to *Journal of Statistical Software*. (LA-UR-20-23587)

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Samsel, F., P. J. J. Wolfram, A. Barres, T. Turton and R. B. Bujack. Colormapping Resources and Strategies for Organized Intuitive Environmental Visualization. Submitted to *Environmental Earth Sciences*. (LA-UR-19-20148)

Tasseff, B. A., R. W. Bent, M. A. Epelman, D. Pasqualini and P. Van Hentenryck. Exact Mixed-integer Convex Programming Formulation for Optimal Water Network Design. Submitted to *INFORMS Journal on Optimization*. (LA-UR-20-27429)

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*Tasseff, B., R. Bent and P. Van Hentenryck. Optimization of Structural Flood Mitigation Strategies. 2019. *Water Resources Research*. **55** (2): 1490-1509. (LA-UR-18-21506 DOI: 10.1029/2018WR024362)

Wang, S., D. Pasqualini, N. M. Urban, C. J. Coffrin, R. W. Bent and S. Mason. An Optimization-Based Adaptation Framework for Coastal Electrical Infrastructure Resilience To Climate Change. Submitted to *Climatic Change*. (LA-UR-19-22145)

Wang, S., R. W. Bent, C. J. Coffrin, S. Eksioglu and S. Mason. A Scenario-Based Algorithm for Joint Chance-Constrained Programs with Finite Support and Feasible Integer Recourse. Submitted to *Computers and Operations Research*. (LA-UR-19-29356)

*Ward, N., B. Bond-Lamberty, V. Bailey, D. Butman, E. Canuel, H. Diefenerfer, N. Ganju, M. Goni, C. Hopkinson, T. Khangaokar, A. Langley, N. G. McDowell, A. Myers-Pigg, R. Neumann, C. Osburn, R. Price, J. C. Rowland, A. Sengupta, M. Simard, M. Tzortziou, R. Vargas, P. Weisenhorn and L. Windham-Myers. Representing the function and sensitivity of coastal interfaces in Earth system models. 2020. *Nature Communications*. **11** (1): 2458. (LA-UR-19-31990 DOI: 10.1038/s41467-020-16236-2)

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Presentation Slides

Cao, Z., S. R. Brus, D. Pasqualini and P. J. J. Wolfram. Predicting Coastal Flooding Under Long-Term Climate Change with MPAS-Ocean. Presented at *2020 AGU meeting*, virtual, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29540)

Francom, D. C., N. M. Urban and D. Pasqualini. Storm Surge Model Emulation and Sensitivity Analysis using Bayesian Adaptive Splines. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-28 - 2019-07-28. (LA-UR-19-27244)

Hunke, E. C., J. C. Rowland, L. Van Roekel, C. B. Begeman and J. P. Schwenk. Selections from LANL's LDRD programs. Presented at *Briefing for DOE/SC/BER program managers*, online, New Mexico, United States, 2020-10-01 - 2020-10-01. (LA-UR-20-27728)

Pasqualini, D. Co-evolution of Coastal Natural and Human-engineered Systems: Making Decisions under uncertainty. Presented at *Complex Natural and Engineered Systems Capabilities Review*, Los Alamos, New Mexico, United States, 2020-09-14 - 2020-09-14. (LA-UR-20-26809)

Pasqualini, D., N. M. Urban, J. C. Rowland, J. D. Moulton, P. J. J. Wolfram, C. Xu, R. W. Bent, D. W. Goodsman, D. C. Francom, H. Nagarajan, B. A. Tasseff, B. Li and B. A. Vega-Westhoff. Preparing Our Coastlines for Climate Security Threats. Presented at *AGU Fall 2018*, Washington, DC, District Of Columbia, United States, 2018-12-10 - 2018-12-15. (LA-UR-18-31515)

Rowland, J. C. ModEx and landsurface processes: Thoughts on matching models, scales, and process-based observations. . (LA-UR-19-29437)

Tasseff, B. A., C. J. Coffrin and R. W. Bent. WaterModels.jl: An Open-source Framework for Exploring Water Network Optimization Formulations. Presented at *2019 INFORMS Annual Meeting*, Seattle, Washington, United States, 2019-10-20 - 2019-10-23. (LA-UR-19-30453)

Tasseff, B. A., R. W. Bent, M. A. Epelman, D. Pasqualini and P. Van Hentenryck. Exact Mixed-integer Convex Programming Formulation for Optimal Water Network Design. Presented at *INFORMS 2020 Annual Virtual Meeting*, Virtual, New Mexico, United States, 2020-11-08 - 2020-11-11. (LA-UR-20-27981)

Tasseff, B. A., R. W. Bent and P. Van Hentenryck. Cutting Planes for Global Optimization of Water Distribution Network Design. Presented at *2019 INFORMS Annual Meeting*, Seattle, Washington, United States, 2019-10-20 - 2019-10-23. (LA-UR-19-30452)

Urban, N. M., A. M. Barthel, R. W. Bent, M. Berdahl, D. S. Comeau, M. Dinniman, D. C. Francom, D. A. S. Foster, M. W. Hecht, A. Jonko, J. Klinck, G. Leguy, B. Li, W. H. Lipscomb, C. Little, J. D. Moulton, B. T. Nadiga, D. Pasqualini, J. C. Rowland, R. Sriver, E. Steig, B. A. Tasseff, C. Veneziani, T. Verma, S. Wang, W. Weijer, P. J. J. Wolfram and C. Xu. Synthesizing climate uncertainties and decision making in complex interdependent coastal systems. Presented at *Sea Level Hotspots from Florida to Maine*, Norfolk, Virginia, United States, 2019-04-23 - 2019-04-23. (LA-UR-19-24103)

Urban, N. M., D. Pasqualini and J. C. Rowland. Coastal energy-water-land interactions and adaptation. Presented at *Energy Modeling Forum: Analyses of Multi-sector Energy and Environmental Dynamics Workshop*, Snowmass, Colorado, United States, 2018-10-18 - 2018-10-18. (LA-UR-18-30324)

Urban, N. M., D. Pasqualini and J. C. Rowland. Adaptation science at LANL: High-fidelity endogenous modeling of coastal energy-water infrastructure adaptation. Presented at *Snowmass Workshop: Analyses of Multi-sector Energy and Environmental Dynamics*, Snowmass, Colorado, United States, 2018-07-18 - 2018-07-18. (LA-UR-18-30187)

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collaborative meeting, Golden, Colorado, United States, 2018-10-04 - 2018-10-04. (LA-UR-18-30331)

J. Wolfram, P. J. Coastal modeling using MPAS-O and E3SM. . (LA-UR-18-29530)

J. Wolfram, P. J. Coastal modeling through novel ocean developments in E3SM. Presented at *DOE Earth and Environmental System Modeling (EESM) PI Meeting*, Poto, Maryland, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30635)

J. Wolfram, P. J. Modeling the land-water interface in the Energy Exascale Earth System Model. Presented at *Toledo Lab Day*, Toledo, Ohio, United States, 2019-10-10 - 2019-10-10. (LA-UR-19-30209)

J. Wolfram, P. J. Multiscale Exascale Earth System Modeling (E3SM): gaining clarity on earth system evolution through mixing across scales in global to coastal ocean modeling. . (LA-UR-19-31491)

J. Wolfram, P. J. Understanding coastal flooding by hurricanes and drought-induced water quality degradation for coastal power and water networks. . (LA-UR-20-22017)

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J. Wolfram, P. J., S. R. Brus, M. R. Petersen, Z. Cao, D. Engwirda, X. S. Asay-Davis, M. E. Maltrud, J. D. Wolfe, A. F. Roberts, T. Zhou, G. Bisht, Z. Tan and R. Leung. Global to coastal ocean modeling in the Energy Exascale Earth System Model. Presented at *The 18th International workshop on Multi-scale (Un)-structured mesh numerical Modeling for coastal, shelf, and global ocean dynamics (IMUM 2019)*, Santa Fe, New Mexico, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-29580)

J. Wolfram, P. J., S. R. Brus, M. R. Petersen, Z. Cao, D. Engwirda, X. S. Asay-Davis, M. E. Maltrud, J. D. Wolfe, A. F. Roberts, T. Zhou, G. Bisht, Z. Tan and R. Leung. Global to Coastal Multiscale Modeling via Land-river-ocean Coupling in the Energy Exascale Earth System Model (E3SM). Presented at *ESCO 2020*, Virtual, New Mexico, United States, 2020-06-08 - 2020-06-11. (LA-UR-20-24263)

J. Wolfram, P. J., S. R. Brus and Z. Cao. Coastal modeling for the Delaware using MPAS-O / E3SM for hurricane and decadal simulation. Presented at *FFMP Workgroup and Salinity group*, Trenton, New Jersey, United States, 2019-04-11 - 2019-04-11. (LA-UR-19-23344)

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Posters

Bent, R. W., B. Li, H. Nagarajan, R. Jiang and J. Mathieu. Decomposition and Cutting-Plane Based Algorithm for Stochastic Climate Adaptation Problem Using Special Order Sets. . (LA-UR-18-27129)

Pasqualini, D., N. M. Urban, J. C. Rowland, P. J. J. Wolfram, J. D. Moulton, C. Xu, R. W. Bent, H. Nagarajan, B. A. Tasseff, D. W. Goodsman and D. C. Francom. Co-evolution of Coastal Natural and Human-Engineered Systems: Making Decisions under Uncertainty. Presented at *ECM15*, Seattle, Washington, United States, 2018-06-25 - 2018-06-28. (LA-UR-18-30410)

Rowland, J. C. and N. M. Urban. Coastal adaptation planning through coastal dynamics modeling, end-to-end uncertainty fusion, and probabilistic design optimization. . (LA-UR-18-22742)

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Zhang, Y. Wetland hydrologic resilience to climate variability: a case study at a coastal wetland of North Carolina, USA. Presented at *American Geophysical Union*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-15. (LA-UR-18-31331)

Zhang, Y. Assessing the hydrologic resilience of coastal wetlands at the Southeastern US under climate disturbances: the critical role of regional-scale hydrologic interaction. Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32008)

Other

Moulton, J. D., E. Coon, S. L. Painter, R. V. Garimella, S. Molins, K. Lipnikov, D. Svyatsky, V. Freedman, D. R. Harp, A. L. Atchley

and Z. Lu. Summary for Amanzi-ATS R&D 100 Video Entry. Audio/Visual. (LA-UR-20-25076)

Pasqualini, D. and D. C. Francom. Storm surge simulation data using SLOSH. Dataset. (LA-UR-20-27106)

BioManufacturing with Intelligent Adaptive Control: BioManIAC

Babetta Marrone
20190001DR

Project Description

Plastics made from petroleum are a mainstay in our daily lives, but the environmental problems they create are driving an urgent search for bio-based alternatives. Currently, over 300 million-metric-tons of plastic are produced worldwide, yet only a fraction is derived from bio-based feedstocks. The biopolymer field suffers from lack of deep understanding of what makes a good bioplastic. Bio-derived molecules have more diverse chemical functionalities than those found in petroleum-based molecules and therefore offer a rich resource for discovering new monomers for synthesis of novel biopolymers for conversion into plastic materials with performance advantages. Microalgae are an attractive bio-feedstock for industrial applications because of their rapid growth and higher productivity-per-unit-land-area than any plant system. We will identify new molecular precursors for bioplastics using microalgae as the feedstock, and develop machine learning (ML) tools to optimize chemical discovery and design. ML will accelerate the development of new biopolymers from algae by efficiently matching large data sets of chemical structures to specific sets of properties and desired functionalities. We will build a chemical knowledge base that will provide the foundation to advance the development of novel biopolymers for the manufacture of plastics for a wide range of applications and optimal end-of-life degradation

Publications

Journal Articles

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Molecular Dynamics Simulations for Glass Transition Temperature Predictions of Polyhydroxyalkanoate Biopolymers. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-20-23226)

Chen, L., G. Pilania, R. Batra, T. D. Huan, C. Kim, C. Kuenneth and R. Ramprasad. Polymer Informatics: Current Status and Critical Next Steps. Submitted to *Materials Science & Engineering R: Reports*. (LA-UR-20-27820)

Gonzalez Esquer, C. R., A. T. Lantz, A. Turmo, C. A. Kerfeld and T. D. Sharkey. Insertion-engineered terpene synthases. Submitted to *Science*. (LA-UR-20-22812)

Marrone, B. L. A letter of encouragement to STEM job seekers, in the time of Coronavirus. Submitted to *Science*. (LA-UR-20-23532)

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Pion-Tonachini, L., K. Bouchard, H. Garcia Martin, S. Peisert, B. Holtz, A. Aswani, D. Dwivedi, H. Wainwright, G. Pilania, B. L. Marrone, N. Falco, M. Prabhat, D. Arnold, A. Wolf-Yadlin, S. Powers, S. Climer, Q. Jackson, T. Carlson, A. Justice, C. Tomlin, D. Jacobson, G. Micklem, G. V. Gkoutos, P. J. Bickel, J. Cazier, J. M&#127;uller, B. Webb-Robertson, R. Stevens, M. Anderson, K. Kreutz-Delgado, M. W. Mahoney and J. B. Brown. Learning from learning machines. Submitted to *Science*. (LA-UR-20-29609)

Vasudevan, R., G. Pilania and P. V. Balachandran. Editorial for the Journal of Applied Physics Special Topic on Machine Learning for Materials Design and Discovery. Submitted to *Journal of Applied Physics*. (LA-UR-20-30189)

Books/Chapters

Pilania, G., P. Balachandra, J. E. Gubernatis and T. Lookman. Data-Based Methods for Materials Design and Discovery Basic Ideas and General Methods. (LA-UR-19-31822)

Presentation Slides

Banerjee, S. Green Feat Disruptech Application. Presented at *Disruptech*, Los Alamos, New Mexico, United States, 2021-02-24 - 2021-02-26. (LA-UR-21-21360)

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Structure-Property Mappings for Bio-Advantaged Polyhydroxyalkanoate (PHA)-based Polymers. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22031)

I. Coleman, C. E., S. F. Lee, N. S. Gupta, K. Lee, C. N. Iverson and J. H. Dumont. BioManIAC: Investigating the degradation of PHB biopolymers and their derivatives. Presented at *LANL 2020 Student symposium*, Los Alamos, New Mexico, United States, 2020-08-21 - 2020-08-21. (LA-UR-20-25407)

Dumont, J. H. Biodegradable polymers for packaging applications. . (LA-UR-21-21543)

Jha, R. K. Synthetic Biology for a Better World.. Presented at *CFO Connect*, Los Alamos, New Mexico, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24201)

Lalonde, J. N., B. L. Marrone and G. Pilania. Applications of machine learning to degradation prediction of poly(hydroxyalkanoates). Presented at *LANL 2020 Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-20 - 2020-08-21. (LA-UR-20-25724)

Marrone, B. L. Sustainability through Biofuels and Bioproducts. Presented at *National Lab Day*, Toledo, Ohio, United States, 2019-10-09 - 2019-11-09. (LA-UR-19-30151)

Marrone, B. L. Alternative Careers in Biology. . (LA-UR-20-27553)

Marrone, B. L. LANL Biological/Biochemical Capabilities and Technologies for\xc2\xa0CO2\xc2\xa0Conversion\xc2\xa0. . (LA-UR-21-21681)

Pilania, G. BioManufacturing with Intelligent Adaptive Control (BioManIAC). . (LA-UR-21-21706)

Uberuaga, B. P. Highlights performed on LANL IC on the project w19_matprops. . (LA-UR-20-22424)

Posters

Gonzalez Esquer, C. R., G. Pilania, N. M. Sudasinghe Appuhamilage, B. A. Parsons, C. R. Steadman, K. Lee, K. Campbell, R. K. Jha, C. N. Iverson, T. Lookman, S. R. Starkenburg, T. T. Dale and B. L. Marrone. Biomanufacturing with Intelligent Adaptive Control. Presented at *13th Workshop on Cyanobacteria*, Boulder, Colorado, United States, 2019-04-06 - 2019-04-09. (LA-UR-19-23867)

Lakis, I. M., P. K. Dighe, C. R. Gonzalez Esquer and B. L. Marrone. Multifactorial Optimization of Cyanobacterial Polymer Production Platforms. Presented at *2019 UGS LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27571)

Obrey, S. J., G. F. Levine and K. Erickson. Modifying Carboxylate-Alumoxane Surfaces with Click Chemistry. Presented at *LANL Annual Student Symposium*, los alamos, New Mexico, United States, 2019-08-06 - 2019-08-08. (LA-UR-19-27227)

Salts in Hot Water – Developing a Scientific Basis for Supercritical Desalination, Strategic Metal Recovery, and Industrial Water Treatment

Robert Currier
20190057DR

Project Description

Fresh water will undoubtedly become an increasingly important aspect of international stability. Fresh water production by thermal desalination with simultaneous recovery of strategic elements offers a route to affordable water and a secure supply of key metals. Deep aquifer brines contain many valuable metals. With China manipulating rare earth element supply and prices, it is important to secure domestic sources of all strategic metals. The co-production of metals with desalination can provide a means of doing so. An integrated process to accomplish these objectives will be developed using inexpensive thermal energy (heat). The process can also impact energy production. Current practice of off-site transport of water co-produces with oil/gas followed by deep well re-injection is costly and can induce earthquakes. Also, sequestration of carbon dioxide in aquifers requires removal of equal volumes of brine to avoid seismicity. Treatment/use of extracted brine would alleviate these concerns and costs. Water also facilitates the migration of heavy metals including actinides and post-detonation fission products. This effort will provide insights into their environmental transport and nuclear material fate during rare, but usually consequential, nuclear accidents. New methods for stabilizing and disposing of hazardous waste streams, and for metal recovery/recycling, are expected.

Publications

Journal Articles

Alcorn, C. D., K. A. Velizhanin, A. C. Strzelecki, H. D. Nisbet, R. C. Roback, R. P. Currier and A. Migdissov. An Experimental Study of the Solubility of Rare Earth Chloride Salts (La, Nd, Er) in HCl Bearing Water Vapor up to 425 \xc2\xb0C. Submitted to *Geochimica et Cosmochimica Acta*. (LA-UR-20-29341)

Maerzke, K. A., T. Yoon, R. B. Jadrich, J. A. Leiding and R. P. Currier. First Principles Simulations of CuCl in High Temperature Water Vapor. Submitted to *Journal of Physical Chemistry B*. (LA-UR-21-20037)

Middleton, R. S., J. M. Bielicki, B. Chen, A. F. Clarens, R. P. Currier, K. M. Ellett, D. R. Harp, B. A. Hoover, R. M. Kammer, D. N. McFarlane, J. D. Ogland- Hand, R. J. Pawar, P. H. Stauffer, H. S. Viswanathan and S. P. Yaw. Great SCO2T! Rapid tool for carbon sequestration science, engineering, and economics. 2020. *Applied Computing and Geosciences*. **7**: 100035. (LA-UR-19-31754 DOI: 10.1016/j.acags.2020.100035)

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Patel, L. A., T. Yoon, R. P. Currier and K. A. Maerzke. NaCl Aggregation in Water at Elevated Temperatures and Pressures: Comparison of Classical Force Fields. Submitted to *Journal of Chemical Physics*. (LA-UR-20-27511)

Sharan, P., S. M. Jaffe, T. Yoon, T. Ju, R. P. Currier and A. T. Findikoglu. Economic Feasibility of Capacitive Deionization: Impact of Brine Disposal and Comparison with Reverse Osmosis. Submitted to *Journal of Cleaner Production*. (LA-UR-20-26776)

Strzelecki, A. C., A. Migdissov, H. Boukhalfa, K. B. Sauer, K. G. McIntosh, R. P. Currier and A. E. Williams-Jones. Fluocerite: The phantom precursor for REE fractionation in natural ore-forming systems. Submitted to *Nature Geoscience*. (LA-UR-19-31633)

Velizhanin, K. A., C. D. Alcorn, A. A. Migdisov and R. P. Currier. Rigorous analysis of non-ideal solubility of sodium and copper chlorides in water vapor using Pitzer-Pabalan model. 2020. *Fluid Phase Equilibria*. **522**: 112731. (LA-UR-20-22702 DOI: 10.1016/j.fluid.2020.112731)

*Yoon, T. J., L. A. Patel, M. J. Vigil, K. A. Maerzke, A. T. Findikoglu and R. P. Currier. Electrical conductivity, ion pairing, and ion self-diffusion in aqueous NaCl solutions at elevated temperatures and pressures. 2019. *Journal of Chemical Physics*. **151** (22): 224504. (LA-UR-19-27151 DOI: 10.1063/1.5128671)

*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*.

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Chu, S. and R. S. Middleton. Summary of Collecting Existing Data on Brines. Unpublished report. (LA-UR-20-26709)

Maerzke, K. A. and L. R. Pratt. Salts in Hot Water: Developing a Scientific Basis for Supercritical Desalination and Strategic Metal Recovery. Unpublished report. (LA-UR-20-26967)

Presentation Slides

Currier, R. P. and A. Migdissov. Salts in Hot Water – Developing a Scientific Basis for Supercritical Desalination, Strategic Metal Recovery, and Industrial Water Treatment. . (LA-UR-20-21500)

Findikoglu, A. T., T. Yoon, M. J. Vigil and P. Sharan. Impedance/Dielectric Spectroscopy and Theory/Engineering Implications. . (LA-UR-20-21743)

Maerzke, K. A. Monte Carlo Simulations of Phase Equilibria and Vapor-Phase Aggregation. . (LA-UR-20-21627)

Maerzke, K. A., L. A. Patel and T. Yoon. Salts in Hot Water: Developing a Scientific Basis for Supercritical Desalination and Strategic Metal Recovery. . (LA-UR-20-21963)

Maerzke, K. A., R. B. Jadrich, T. Yoon, J. A. Leiding and R. P. Currier. First Principles Simulations of CuCl in High Temperature Water Vapor. Presented at *Telluride Science Lecture Series*, Los Alamos, New Mexico, United States, 2020-08-07 - 2020-08-07. (LA-UR-20-25990)

Middleton, R. S. SimCCS: development and Applications. Presented at *NETL Annual Meeting and Pittsburgh Coal Conference*, Pittsburgh, Pennsylvania, United States, 2020-09-08 - 2020-09-08. (LA-UR-20-26707)

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Singh, R. P. Advanced materials and technologies for FEWS. Presented at *Regional academic collaborations initiative (ReACt) Workshop on Food Energy Water Systems*, Las Cruces, New Mexico, United States, 2019-08-13 - 2019-08-14. (LA-UR-19-28119)

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Vigil, M. J. Development of Electrochemical Methods for In Situ Diagnostics of Fluids: Impedance Spectroscopy and Cyclic Voltammetry - Script. Presented at *2020 symposium presentation*, Los Alamos, New Mexico, United States, 2020-08-03 - 2020-08-03. (LA-UR-20-25404)

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Posters

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Riglin, J. D., P. Sharan, T. Yoon, A. T. Findikoglu and R. P. Currier. Process Design & Engineering. . (LA-UR-20-21744)

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

Gian Delzanno
20200073DR

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).

Publications

Journal Articles

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Colestock, P., G. L. Delzanno and N. Yampolsky. Thermal Mode Radiation from VLF Antennas in the Inner Magnetosphere. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-21-20127)

Colpitts, C. A., Y. Miyoshi, Y. Kasahara, J. R. Wygant, C. Cattell, A. Breneman, C. A. Kletzing, G. S. Cunningham, G. L. Delzanno, M. Hikishima, S. Matsuda, Y. Katoh, J. F. Ripoll, I. Shinohara and A. Matsuoka. First Direct Observations of Propagation of Discrete Chorus Elements From the Equatorial Source to Higher Latitudes, Using the Van Allen Probes and Arase Satellites. 2020. *Journal of Geophysical Research: Space Physics*. **125** (10): e2020JA028315. (LA-UR-20-24874 DOI: 10.1029/2020JA028315)

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Delzanno, G. L., J. E. Borovsky and E. Mishin. Editorial: Active Experiments in Space: Past, Present, and Future. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-20609 DOI: 10.3389/fspas.2020.00005)

Ghaffari, R., C. M. Cully, D. L. Turner and G. D. Reeves. Characteristics of Electron Precipitation during 40 Energetic Electron Injections Inferred via Subionospheric VLF Signal Propagation. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-20-24385)

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Pierrard, V., J. F. Ripoll, G. S. Cunningham, E. Botek, O. Santolik, S. A. Thaller, W. S. Kurth, C. A. Kletzing and M. Cosmides. Observations and simulations of dropout events and flux enhancements in October 2013: Comparing MEO equatorial with LEO polar orbit. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-20-27453)

D. Reeves, E. G. Earth's Radiation Belts: The Hazards to Satellites and What Can Be Done to Mitigate the Risks?. Submitted to *Proceedings of the AMOS conference*. (LA-UR-20-26784)

D. Reeves, E. G., G. L. Delzanno, P. A. Fernandes, K. Yakymenko, B. E. Carlsten, J. W. I. Lewellen, M. A. Holloway, D. C. Nguyen, R. F. Pfaff, W. M. Farrell, D. Rowland, M. Samara, E. Sanchez, E. Spanswick, E. Donovan and V. Roytershteyn. The Beam Plasma Interactions Experiment: An Active Experiment using Pulsed Electron Beams. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-24628)

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Defining Radiation Belt Enhancement Events Based on Probability Distributions. 2020. *Space Weather*. **18** (8): e2020SW002528. (LA-UR-20-24379 DOI: 10.1029/2020SW002528)

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Cowee, M. and X. Fu. Plasma Waves and Structures in the Inner Magnetosphere – Institutional Computing 2020. . (LA-UR-21-22167)

Cunningham, G. S. High-latitude electron beam effective for remediating an artificial belt at IRIDIUM!. . (LA-UR-20-21935)

Delzanno, G. L. RBR-ACES November 2019. . (LA-UR-19-31629)

Delzanno, G. L. Spacecraft charging studies. . (LA-UR-19-32262)

Delzanno, G. L. LANL-DSX collaboration. . (LA-UR-20-25946)

Delzanno, G. L. New coupling between whistler waves and cold plasmas. . (LA-UR-21-20154)

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Delzanno, G. L., Q. R. Marksteiner, E. G. D. Reeves, J. M. Broll, B. E. Carlsten, P. Colestock, M. Cowee, G. S. Cunningham, L. D. Duffy, X. Fu, C. A. M. Jeffery, K. A. Shipman, D. Svyatsky, N. Yampolsky, J. M. Albert, C. Crabtree, S. Dorfman, J. McCollough and V. Roytershteyn. Recent progress towards a radiation belt remediation strategy based on artificial injection of plasma waves. . (LA-UR-20-26764)

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Delzanno, G. L., V. Roytershteyn, P. Colestock and J. C. Holmes. The impact of cold electrons on whistler waves. . (LA-UR-21-20394)

Delzanno, G. L. and V. Roytershteyn. Cold electrons and whistler waves. Presented at *Mini-GEM Workshop*, Online, District Of Columbia, United States, 2021-01-20 - 2021-01-20. (LA-UR-21-20447)

Duffy, L. D. Electron Beam Dynamics in Propagation. Presented at *Radiation Belt Remediation DR Appraisal meeting*, Los Alamos, New Mexico, United States, 2021-01-12 - 2021-01-12. (LA-UR-21-20134)

Fu, X., G. S. Cunningham, M. Cowee and E. G. D. Reeves. Effects of Artificial Whistler Waves on MeV Electrons: Test-Particle Simulations. . (LA-UR-21-20145)

Holmes, J. C., G. L. Delzanno, P. L. Colestock, C. A. M. Jeffery, E. G. D. Reeves, K. Yakymenko, O. Koshkarov and Q. R. Marksteiner. Wave propagation with ray tracing. . (LA-UR-21-20183)

D. Reeves, E. G. Earth’s Radiation Belts The Hazards to Satellites and \xe2\x80\xa8What Can Be Done to Mitigate the Risks?. Presented at *Advanced Maui Optical Surveillance (AMOS) - Virtual*, Virtual, Hawaii, United States, 2020-09-15 - 2020-09-15. (LA-UR-20-26903)

D. Reeves, E. G. RBR-ACES Validation Activities. . (LA-UR-21-20289)

D. Reeves, E. G., G. L. Delzanno, Q. R. Marksteiner, G. S. Cunningham, M. Cowee, M. A. Holloway, R. M. Holmes and P. A. Fernandes. Exploiting Our New Understanding of Wave- Particle Interactions to EvaluateTechniques for Radiation Belt Remediation. Presented at *COSPAR*, Sidney, Australia, 2021-01-28 - 2021-01-28. (LA-UR-20-30307)

Yampolsky, N., K. A. Shipman, P. L. Colestock, Q. R. Marksteiner and G. L. Delzanno. Generation of waves in magnetized plasma. . (LA-UR-20-20786)

Directed Plant-Microbiome Evolution for Food and Biofuel Security

Sanna Sevanto
20200109DR

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 and. 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.

Publications

Journal Articles

Fawcett, P. J., R. S. Anderson, E. T. Brown, J. P. Werne, S. Contreras, S. Smith, J. M. Heikoop and C. D. Allen. Millennial-Scale Climate Change During a Mid-Pleistocene Glacial (MIS 12): A Lacustrine Record from the Valles Caldera, NM. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-24162)

Nakad, M., T. Witelski, J. Domec, S. A. Sevanto and G. Katul. Taylor dispersion in osmotically driven laminar flows in phloem. Submitted to *Journal of Fluid Mechanics*. (LA-UR-20-23039)

*Sevanto, S. Why do plants have waxy leaves? Do we know after all?. 2020. *Tree Physiology*. **40** (7): 823-826. (LA-UR-19-30922 DOI: 10.1093/treephys/tpz117)

Sevanto, S. A., C. Grossiord, T. Klein and S. Reed. Editorial for the Research Topic: Plant-Soil Interactions under Changing World. Submitted to *Frontiers in Plant Science*. (LA-UR-20-27969)

Presentation Slides

Dickman, L. T., E. R. Lathrop, J. P. Heneghan, D. Musa, M. Ryan and S. A. Sevanto. Water availability shifts stomatal thresholds. Presented at *Ecological Society of America*, Salt Lake City, Utah, United States, 2020-08-03 - 2020-08-03. (LA-UR-20-25496)

Sevanto, S. A. Good and bad microbes, and good and bad stress –from plant perspective. . (LA-UR-20-27377)

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)

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)

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

Jacob Spendelow
20200200DR

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.

Publications

Journal Articles

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)

*Kim, D., S. H. R. Shin, Y. Kim, K. Crossley, Y. Kim, H. Han and J. Yoo. Hierarchical assembly of ZnO nanowire trunks decorated with ZnO nanosheets for lithium ion battery anodes. 2020. *RSC Advances*. **10** (23): 13655-13661. (LA-UR-19-28270 DOI: 10.1039/D0RA00372G)

Kim, D., T. Ahmed, K. W. Crossley, J. K. S. Baldwin, Y. Kim, C. J. Sheehan, N. Li, D. Pete and J. Yoo. Improving the performances of Si nanowire-based lithium ion battery anodes by suppressed Au diffusion on TiN. Submitted to *ACS Applied Nano Materials*. (LA-UR-19-20571)

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Presentation Slides

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

de Melo Kort-Kamp, W. J. and A. Rahman. Structured electrodes DR - Theory team update. Presented at *DR Regular Meeting*, Los Alamos, New Mexico, United States, 2021-01-05 - 2021-01-05. (LA-UR-21-20055)

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)

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)

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)

Establishing a Radiotherapeutic Capability to Counter Biothreats

Stosh Kozimor
20180005DR

Project Description

Our proposed work directly supports our national security by developing and validating a novel, countermeasure pipeline against antimicrobial and multi-drug resistant bacterial pathogens. To protect our nation's health, we are offering a therapeutic alternative to the declining effectiveness of antibiotics. To maintain our national security and protect our nation's warfighters, we are demonstrating a rapid radiotherapies capability to combat bacterial pathogens developed as multi-drug resistant bioweapons.

Technical Outcomes

This project successfully established a capability to counter biothreats using radiotherapies. Antibodies selective for Y. pestis were developed and the team demonstrated actinium (Ac)-225 could be used in vitro to kill Y. pestis. The team characterized the first chelated Ac complex, solutions behavior of Ac reagents used for chelation, and established a computer assisted chelator design concept for Ac.

Publications

Journal Articles

Aldrich, K. E., S. A. Kozimor, I. A. Popov, E. R. Batista, P. Yang, V. Mocko, B. Stein, L. M. Lilley, S. M. Greer, M. Y. Livshits and M. T. Janicke. Synthesis, Solid-State, and Solution Characterization of an “In-Cage” Scandium-NOTA Complex. Submitted to *Inorganic Chemistry*. (LA-UR-21-22369)

*Ferrier, M. G., B. Stein, S. E. Bone, S. K. Cary, A. S. Ditter, S. A. Kozimor, J. S. Lezama Pacheco, V. Mocko and G. T. Seidler. The coordination chemistry of Cm , Am , and Ac in nitrate solutions: an actinide L -edge EXAFS study. 2018. *Chemical Science*. **9** (35): 7078-7090. (LA-UR-18-22688 DOI: 10.1039/C8SC02270D)

Jones, Z. R., M. Y. Livshits, F. D. J. White, E. Danielou Dalodiere, M. G. Ferrier, L. M. Lilley, K. K. Knope, S. A. Kozimor, V. Mocko, B. Stein, J. N. Wacker and D. H. Woen. Advancing Understanding of Actinide(III) (Ac, Am, Cm) Coordination Chemistry in Ammonium Acetate and Acetic Acid Buffered Aqueous Stock Solutions. Submitted to *Journal of the American Chemical Society*. (LA-UR-20-30210)

Kozimor, S. A., K. E. Aldrich, C. Eiroa Lledo, L. M. Lilley, V. Mocko, B. Stein and N. H. Lam. PREPARATION OF AN ACTINIUM-228 GENERATOR. Submitted to *Inorganic Chemistry*. (LA-UR-19-31448)

Kozimor, S. A. and R. J. Abergel. Preface for the Forum on Innovative f-element Chelating Strategies. Submitted to *Inorganic Chemistry*. (LA-UR-19-32400)

Lilley, L. M., M. Y. Livshits, K. E. Aldrich, L. R. Stromberg, B. Stein, G. L. Wagner, M. T. Janicke, H. Mukundan, S. A. Kozimor, N. H. Lam and R. J. Abergel. Revisiting ThIV-Desferrioxamine: Characterization of a Fluorescent Bacterial Probe. Submitted to *ACS Central Science*. (LA-UR-20-24508)

Lillo, A. M., N. Velappan, A. J. Watts, M. E. Phipps, R. J. Abergel and M. Flick. Affinity matured anti-Y. pestis F1 antigen human antibodies and their potential diagnostic and therapeutic applications. Submitted to *Bioconjugate Chemistry*. (LA-UR-21-20529)

Lillo, A. M., N. Velappan, J. M. Kelliher, A. J. Watts, S. Merriman, G. Vuyisich, L. M. Lilley, K. E. Coombs, T. Mastren, M. Teshima, B. Stein, G. L. Wagner, S. Iyer, A. M. Bradbury, J. F. Harris, A. E. K. Dichosa and S. A. Kozimor. Development of Anti-Yersinia pestis Human Antibodies with Features Required for Diagnostic and Therapeutic Applications. 2020. *ImmunoTargets and Therapy*. **9**: 299-316. (LA-UR-20-30360 DOI: 10.2147/ITT.S267077)

Morgenstern, A. L., L. M. Lilley, B. Stein, S. A. Kozimor, E. R. Batista and P. Yang. Computer-Assisted Design of Macrocyclic Chelators for Actinium- 225 Radiotherapeutics. Submitted to *Chemical Science*. (LA-UR-20-25129)

Stein, B., A. L. Morgenstern, E. R. Batista, E. R. Birnbaum, S. E. Bone, S. K. Schrell, M. G. Ferrier, K. D. John, J. L. Pacheco, S. A. Kozimor, B. L. Scott, V. Mocko and P. Yang. Chelating +3 Metals (Ac, Am, Cm, La) with H8DOTP; 1,4,7,10-Tetraazacyclododecane-1,4,7,10-Tetra(methylene) Phosphonic Acid. Submitted to *Nature Chemistry*. (LA-UR-19-25974)

Velappan, N., D. Close, L. Hung, L. Naranjo, C. Hemez, N. DeVore, A. M. Lillo and A. R. Bradbury. Construction, characterization and crystal structure of a fluorescent

single-chain Fv chimera. 2021. *Protein Engineering, Design and Selection*. **34**: gzaa029. (LA-UR-20-22202 DOI: 10.1093/protein/gzaa029)

*Woen, D. H., C. Eiroa-Lledo, A. C. Akin, N. H. Anderson, K. T. Bennett, E. R. Birnbaum, A. V. Blake, M. Brugh, E. Dalodiere, E. F. Dorman, M. G. Ferrier, D. K. Hamlin, S. A. Kozimor, Y. Li, L. M. Lilley, V. Mocko, S. L. Thiemann, D. S. Wilbur and F. D. White. A Solid-State Support for Separating Astatine-211 from Bismuth. 2020. *Inorganic Chemistry*. **59** (9): 6137-6146. (LA-UR-19-31728 DOI: 10.1021/acs.inorgchem.0c00221)

Presentation Slides

Delzanno, G. L. Radiation Belt Remediation: A Complex Engineered System (RBR-ACES). . (LA-UR-18-30975)

K. Dichosa, A. E., N. Velappan, L. M. Lilley, S. A. Kozimor and A. M. Lillo. de novo Antibody Selection for Targeted Radiotherapies against AMR Bacterial Pathogens. Presented at *DTRA CBDST Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-31326)

Lilley, L. M. Pipe RAiD. Presented at *Keiretsu angel investor meeting*, San Francisco, California, United States, 2018-11-13 - 2018-11-16. (LA-UR-18-30693)

Lilley, L. M. NAcX Winning the War on Bugs. Presented at *1millionCups*, Denver, Colorado, United States, 2019-03-18 - 2019-03-21. (LA-UR-19-22412)

Lillo, A. M. Nature-inspired Affinity Reagents for On-Demand Sensitive, Specific, Multiplexable, and Fieldable Diagnostics. Presented at *Tech Watch visit with DTRA*, Washington DC, District Of Columbia, United States, 2019-07-01 - 2019-07-01. (LA-UR-19-25911)

Moore, S. C., L. M. Lilley and H. Mukundan. Sabotaging Iron Metabolism: How we can use siderophores as radiotherapeutics against emerging pathogenic threats. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25765)

Morgenstern, A. L. Designing Chelating Agents for Radiotherapeutics. Presented at *Science in "3"*, Los Alamos, New Mexico, United States, 2018-06-13 - 2018-06-13. (LA-UR-18-25063)

Morgenstern, A. L. Design of macrocyclic chelating agents with actinium for development of targeted radiotherapy. Presented at *Sagamore XIX*, Halifax, Canada, 2018-07-08 - 2018-07-13. (LA-UR-18-26089)

Morgenstern, A. L., E. R. Batista, S. A. Kozimor, L. M. Lilley, B. Stein and P. Yang. Bonding analysis of macrocyclic chelating agents with actinium for development of targeted radiotherapy. Presented at *Second European Symposium on Chemical Bonding*, Oviedo, Spain, 2018-09-03 - 2018-09-07. (LA-UR-18-22813)

Morgenstern, A. L., L. M. Lilley, B. Stein, S. A. Kozimor, E. R. Batista and P. Yang. Computational Design of Actinium Chelators for Use in Radiotherapy. Presented at *LDRD Annual Review (20180005DR)*, Los Alamos, New Mexico, United States, 2019-01-14 - 2019-01-14. (LA-UR-19-20099)

Morgenstern, A. L., L. M. Lilley, B. Stein, S. A. Kozimor, E. R. Batista and P. Yang. Computational Design of Actinium-225 Chelators for Targeted Alpha Therapy. Presented at *National ACS Spring Meeting*, Orlando, Florida, United States, 2019-03-30 - 2019-03-30. (LA-UR-19-22744)

Morgenstern, A. L., L. M. Lilley, E. R. Batista, S. A. Kozimor, B. Stein and P. Yang. Computational Design of Actinium Chelators for Use in Radiotherapy. Presented at *Annual Review for LDRD 20180005DR*, Los Alamos, New Mexico, United States, 2019-01-14 - 2019-01-14. (LA-UR-19-20176)

Mukundan, H. Amphiphilic Biomarkers: Discovery, Detection, Measurement, Modeling and Use. . (LA-UR-20-27277)

Mukundan, H. Amphiphilic Biomarkers: DISCOVERY DETECTION MODELING AND USE. Presented at *AMPHIPHILIC BIOMARKERS -DISCOVERY DETECTION MODELING AND USE*, LOS ALAMOS, New Mexico, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-28093)

Mukundan, H. Intelligent Immunity. Presented at *DTRA Promise Workshop*, virtual, District Of Columbia, United States, 2021-01-29 - 2021-01-29. (LA-UR-21-20014)

Stein, B. Actinium's Fight Against Cancer: Alpha Emitting Radioisotopes in Medicine. . (LA-UR-17-30899)

Stein, B. Spectroscopic Studies of Actinium Coordination Chemistry. Presented at *Inorganic Chemistry GRS*, Biddeford, Maine, United States, 2018-06-16 - 2018-06-17. (LA-UR-18-25251)

Stromberg, L. R. Interfacing Biomarkers and Materials Science: applications for detection and therapeutics. Presented at *Seminar for Chemical & Biological Signature Science Group at PNNL*, Richland, Washington, United States, 2021-01-13 - 2021-01-13. (LA-UR-21-20042)

Posters

Coombs, K. E. Development of Radiolabeled Antibody of Plague on an Artificial Lung in vitro. Presented at *CBDS&T DTRA Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-31500)

Coombs, K. E., E. Z. Alipio Lyon, M. O. Ishak, J. M. Kelliher, Y. Shou, A. E. K. Dichosa, P. Nath, J. F. Harris, G. Vuyisich and L. M. Lilley. Development of Radiolabeled Antibody for Radiotherapy of Plague on an Artificial Lung in vitro. . (LA-UR-19-20092)

Kelliher, J. M. and G. Vuyisich. Testing the efficacy of five viability assessment kits for use in targeted radiotherapeutic kill studies. . (LA-UR-19-20043)

Lillo, A. Towards development of "resistance-proof" radio-immuno therapeutics and diagnostics against Yersinia pestis. . (LA-UR-18-26484)

Lillo, A. M. Development of a Resistance-proof Radioimmuno-Antibiotic Cocktail Against Plague. Presented at *16th Discovery on Target Conference*, Boston, Massachusetts, United States, 2018-09-25 - 2018-09-28. (LA-UR-18-28906)

Lillo, A. M. Development of Radioimmunotherapeutics Against Y. pestis. Presented at *2018 ISDCI Conference*, Santa, New Mexico, United States, 2018-06-17 - 2018-06-23. (LA-UR-18-25248)

Lillo, A. M. Towards development of radioimmuno antibiotics: selecting the right anti-Y. pestis and anti-P. aeruginosa antibodies for the job. Presented at *Antibody Engineering & Therapeutics*, San Diego, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32207)

Root, H. D., F. D. J. White, V. Mocko, S. A. Kozimor and J. L. Sessler. Expanded Porphyrins and their f-Element Complexes. Presented at *LANL Annual Student Symposyum*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-26880)

Stein, B., M. Ferrier, S. A. Kozimor, E. R. Batista, P. Yang, A. L. Morgenstern and V. Mocko. Spectroscopic Studies of Actinium Coordination Chemistry. Presented at *Inorganic Chemistry Gordon Research Conference*, Biddeford, Maine, United States, 2018-06-16 - 2018-06-22. (LA-UR-18-25112)

Stein, B., S. A. Kozimor, M. G. Ferrier, J. M. Berg, K. D. John, V. Mocko and E. R. Birnbaum. Spectroscopic Studies of Actinium Coordination Chemistry. . (LA-UR-17-30560)

Stein, B., S. A. Kozimor, V. Mocko, A. L. Morgenstern, P. Yang, E. R. Batista and M. G. Kerlin. Spectroscopic Studies of Actinium Coordination Chemistry. Presented at *DOE BES Heavy Element Chemistry PI Meeting*, Gaithersburg, Maryland, United States, 2019-04-15 - 2019-04-17. (LA-UR-19-23703)

Stromberg, L. R., A. S. Anderson, J. K. Banh, L. Prasad, L. M. Lilley, K. D. Rector, S. A. Kozimor and H. Mukundan. Functionalized Surfaces for Determination of Capture Ligand Affinity and Bacterial Viability. . (LA-UR-19-20244)

Stromberg, L. R., L. M. Lilley, G. L. Wagner, P. K. Dighe, S. A. Kozimor and H. Mukundan. Alpha-emitting 227-Th Complexes for Targeted Cell Death of Pseudomonas aeruginosa. Presented at *ASM/ESCMID Conference on Drug Development to Meet the Challenge of Antimicrobial Resistance*, Boston, Massachusetts, United States, 2019-09-03 - 2019-09-06. (LA-UR-19-28617)

Velappan, N., S. P. Merriman, A. E. K. Dichosa, A. M. Bradbury and A. M. Lillo. Developing anti-Plague Antibodies: Epitope Binning and Affinity Maturation. Presented at *Antibody Engineering and Therapeutics Conference*, San Diego, California, United States, 2019-12-09 - 2019-12-20. (LA-UR-19-32206)

Velappan, N. and A. M. Lillo. AFFINITY MATURATION OF ANTI-F1v ANTIBODIES. Presented at *LDRD review*, Los Alamos, New Mexico, United States, 2019-01-14 - 2019-01-14. (LA-UR-18-31896)

Velappan, N. and A. M. Lillo. AFFINITY MATURATION OF ANTI-F1V ANTIBODIES. . (LA-UR-19-20085)

An Integrated Scaling Approach for Human, Mosquito, and Environment Toward Process-based Disease Prediction

Carrie Manore
20200033DR

Project Description

As part of the Laboratory's global security mission, this project will provide proof-of-concept work demonstrating our ability to forecast human-natural systems as they relate to human health and infectious disease spread with heterogeneous data streams at multiple scales. With increased forecasting capabilities, national and international agencies will have more lead time for resource allocation and mitigation and will be better able to issue appropriate warnings for the public when outbreaks are imminent.

Technical Outcomes

This project made critical advances in scaling mosquito habitat units so that we can couple mosquito population dynamics models with Earth Systems models, while also capturing new mosquito data to create new mosquito distribution maps that have not been updated since the 1980's. These advances will pave the way for an accurate continental-scale model for mosquito-borne diseases.

Publications

Journal Articles

Bartlow, A. W., C. Machalaba, W. Karesh and J. M. Fair. Biodiversity and Global Health: Intersection of Health, Security and the Environment. Submitted to *Med One*. (LA-UR-19-32341)

Castro, L. A., E. N. A. Generous, W. Luo, A. Pastore y Piontti, K. M. Martinez, M. F. Gomes, D. A. Osthus, A. Ziemann, G. Fairchild, A. Vespignani, M. Santillana, C. A. Manore and S. Y. Del Valle. Using heterogeneous data to identify signatures of dengue outbreaks at fine spatial-temporal scales across Brazil. Submitted to *PLOS Neglected Tropical Diseases*. (LA-UR-20-29637)

Manore, C. A., K. C. Kempfert, K. Martinez, A. S. Siraj, J. R. Conrad, L. A. Castro, D. A. Osthus, E. N. A. Generous, N. K. Parikh, G. Fairchild, A. Ziemann and S. Y. Del Valle. Heterogeneous Data Fusion of Time Series to Nowcast Dengue at the State Level in Brazil. Submitted to *ArXiV*. (LA-UR-20-21471)

Conference Papers

DeMets, S. A., A. Ziemann, C. A. Manore and C. Russell. Improving mosquito population predictions in the Greater Toronto Area using remote sensing imagery. Presented at *IEEE Southwest Symposium on Image Analysis and Interpretation (SSIAI)*. (Santa Fe, New Mexico, United States, 2020-03-30 - 2020-03-30). (LA-UR-20-22587)

DeMets, S. A., A. Ziemann, C. A. Manore and C. Russell. Too big, too small, or just right? The influence of multispectral image size on mosquito population predictions in the Greater Toronto Area. Presented at *SPIE Defense and Commercial Sensing*. (Anaheim, California, United States, 2020-04-27 - 2020-05-01). (LA-UR-20-23662)

Presentation Slides

Manore, C. A., K. C. Kempfert, N. K. Parikh, G. Fairchild, A. Ziemann, A. Saij, D. A. Osthus, K. Martinez, L. A. Castro, E. N. A. Generous and S. Y. Del Valle. Unlocking the Predictive Power of Heterogeneous Data to Build an Operational Dengue Forecasting System. Presented at *University of California, San Francisco*, San Francisco, California, United States, 2019-12-03 - 2019-12-03. (LA-UR-19-31828)

Manore, C. A., K. C. Kempfert, N. K. Parikh, G. Fairchild, A. Ziemann, A. Saij, D. A. Osthus, K. Martinez, L. A. Castro, E. N. A. Generous and S. Y. Del Valle. Unlocking the Predictive Power of Heterogeneous Data to Build an Operational Dengue Forecasting System. Presented at *Promoting Research in Social Media and Health Symposium (PRISM)*, San Francisco, California, United States, 2019-12-06 - 2019-12-06. (LA-UR-19-31827)

Posters

DeMets, S. A., A. Ziemann and C. A. Manore. Forecasting mosquito populations in the Greater Toronto Area using multispectral remote sensing imagery. Presented at *Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21566)

Visualizing and Understanding Complex Fluid Transport in 3-Dimensional Microstructure

Hari Viswanathan
20180151ER

Project Description

Flow through fractures is critical for national security applications such as nuclear nonproliferation. Fractures act as the superhighways of flow in the subsurface and characterizing fracture flow is critical for predicting gas seepage from underground nuclear tests from other nation states.

Publications

Journal Articles

*Bakhshian, S., M. Murakami, S. A. Hosseini and Q. Kang. Scaling of Imbibition Front Dynamics in Heterogeneous Porous Media. 2020. *Geophysical Research Letters*. **47** (14): e2020GL087914. (LA-UR-20-22139 DOI: 10.1029/2020GL087914)

*Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Inertial Effects During the Process of Supercritical CO Displacing Brine in a Sandstone: Lattice Boltzmann Simulations Based on the Continuum-Surface-Force and Geometrical Wetting Models. 2019. *Water Resources Research*. **55** (12): 11144-11165. (LA-UR-19-23236 DOI: 10.1029/2019WR025746)

Gong, Y., M. Z. S. Mehana, I. El-monier and H. S. Viswanathan. Proppant Placement in Complex Fracture Geometries: A Computational Fluid Dynamics. Submitted to *Scientific Reports*. (LA-UR-19-29884)

S. Mehana, M. Z., S. Hosseini, T. A. Meckel and H. S. Viswanathan. Modelling the Carbon Dioxide Plume Using Modified-Invasion-Percolation Simulation. Submitted to *Transport in Porous Media*. (LA-UR-19-26910)

*Nguyen, P., J. W. Carey, H. S. Viswanathan and M. Porter. Effectiveness of supercritical-CO2 and N2 huff-and-puff methods of enhanced oil recovery in shale fracture networks using microfluidic experiments. 2018. *Applied Energy*. **230**: 160-174. (LA-UR-18-30569 DOI: 10.1016/j.apenergy.2018.08.098)

Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, D. Derome and J. Carmeliet. Lattice Boltzmann modeling of heat conduction enhancement by colloidal nanoparticle deposition in micro-porous structures. Submitted to *Physical Review E*. (LA-UR-20-22138)

Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, J. Carmeliet and D. Derome. Three influential factors on colloidal nanoparticle deposition for heat conduction enhancement in 3D chip stacks. 2021. *Applied Thermal Engineering*. 116585. (LA-UR-20-23176 DOI: 10.1016/j.applthermaleng.2021.116585)

Ryan, D. P., Y. Chen, P. Nguyen, P. M. Goodwin, J. W. Carey, Q. Kang, J. H. Werner and H. S. Viswanathan. 3D particle transport in multichannel microfluidic networks with rough surfaces. 2020. *Scientific Reports*. **10** (1): 13848. (LA-UR-20-22718 DOI: 10.1038/s41598-020-70728-1)

Ryan, D. P., Y. Chen, T. P. Nguyen, P. M. Goodwin, J. W. Carey, Q. Kang, J. H. Werner and H. S. Viswanathan. Go with the flow: 3D tracking and particle transport within complex fractured networks. Submitted to *Lab on A Chip*. (LA-UR-19-30100)

Presentation Slides

Chen, Y. code performance chart. . (LA-UR-19-21169)

Chen, Y. Recent progresses in image-based pore-scale multiphase flow simulations using advanced models and GPU acceleration. Presented at *Los Alamos - Arizona Days*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-19. (LA-UR-20-23629)

Chen, Y. microfluidic flow animation for AGU fall meeting. Presented at *AGU 2020 fall meeting*, online, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29678)

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Pore-scale Simulation of Residual Trapping of Supercritical CO2 via Cyclic Injections. Presented at *Interpore 10th Annual Meeting*, New Orleans, Louisiana, United States, 2018-05-14 - 2018-05-17. (LA-UR-18-24118)

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Video Clips of Pore-scale Multiphase Flow Simulations in Porous Media. . (LA-UR-18-24814)

Chen, Y., H. S. Viswanathan and Q. Kang. Images of pore-scale LBM simulations. . (LA-UR-18-30193)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. animations that accompany my AGU poster. Presented at *2019 AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32164)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. A new generation of lattice Boltzmann code for pore-scale simulation of multiphase flow in complex geometry with consideration of inertial effects. Presented at *Computational Methods in Water Resources XXIII*, Los Alamos, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30150)

Chen, Y., Q. Kang, H. S. Viswanathan and A. J. Valocchi. A new generation of lattice Boltzmann code for pore-scale simulation of scCO2-brine displacement in complex geometries. Presented at *Interpore 2020*, Los Alamos, New Mexico, United States, 2020-08-31 - 2020-08-31. (LA-UR-20-26550)

Kang, Q., Y. Chen and A. J. Valocchi. Final Report of Institutional Computing Project w19_porescale: Figures. . (LA-UR-20-21775)

Ryan, D. P., J. H. Werner, H. S. Viswanathan, P. M. Goodwin, J. W. Carey, T. P. Nguyen, Y. Chen and Q. Kang. Particle Transport in Fractured Networks:3D Tracking for Observing Surface-particle and Fluid-particle Interactions. Presented at *2019 American Geophysical Union Annual Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32522)

Viswanathan, H. S. dfnWorks Applications: Hydraulic Fracturing, Nuclear Waste Disposal and Nuclear Nonproliferation. Presented at *dfnWorks Workshoip*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29441)

Viswanathan, H. S., D. P. Ryan, Y. Chen, Q. Kang, T. P. Nguyen and J. H. Werner. Microfluidics Experiments and Lattice Boltzmann Simulations to Characterize Multi-phase Flow and Particle Transport in Fracture Networks. Presented at *Interpore*, Valencia, Spain, 2019-05-06 - 2019-05-10. (LA-UR-19-24072)

Viswanathan, H. S. and J. W. Carey. Mechanistic Approach to Analyzing and Improving Unconventional Hydrocarbon Production. . (LA-UR-19-22101)

Posters

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Direct Numerical Simulation of Supercritical CO2 Displacing Brine in a Sandstone: the Importance of Inertial Effects. . (LA-UR-19-28527)

Chen, Y., J. D. Hyman, Q. Kang and H. S. Viswanathan. Comprehensive Numerical Study of Fluid Displacement in Homogeneous/Heterogeneous Microstructures with Consideration of Inertial Effect. Presented at *AGU 2020 fall meeting*, online, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29673)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. Inertial Effects during the Process of scCO2 Displacing Brine in a Sandstone. Presented at *2019 AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32161)

Ryan, D. P., J. H. Werner, T. P. Nguyen, Y. Chen, H. S. Viswanathan, Q. Kang and J. W. Carey. 3D Proppant Tracking through Fracture Networks. Presented at *CINT Triannual Review*, Los Alamos, New Mexico, United States, 2019-05-13 - 2019-05-13. (LA-UR-19-24206)

Ryan, D. P., T. P. Nguyen, Q. Kang, J. W. Carey, H. S. Viswanathan and J. H. Werner. 3D Tracking of Proppants through Fractured Microchannel Networks. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28840)

Ryan, D. P., Y. Chen, T. P. Nguyen, Q. Kang, J. W. Carey, P. M. Goodwin, H. S. Viswanathan and J. H. Werner. Particle Transport in Fractured Networks. Presented at *Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28610)

Other

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Fluid phase distribution data obtained in our 3D direct numerical simulations. Dataset. (LA-UR-19-29828)

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Simulation data of supercritical CO\xc2\xac\xc2\xac2 and brine displacement in a micromodel and sandstone. Dataset. (LA-UR-21-22268)

Chen, Y., J. D. Hyman, Q. Kang and H. S. Viswanathan. Simulation data of fluid displacement in 2D micromodels under different conditions. Dataset. (LA-UR-21-22269)

Chen, Y., J. D. Hyman, Q. Kang and H. S. Viswanathan. Simulation data of supercritical CO2 and brine co-injection to a microfluidic cell. Dataset. (LA-UR-21-22270)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. Simulation data of fluid displacement in sandstones under different conditions. Dataset. (LA-UR-21-22271)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. Simulation data of fluid displacement in sandstone near entire-core scale. Dataset. (LA-UR-21-22272)

Chen, Y., Q. Kang and H. S. Viswanathan. Simulation data of particle transport in a microfluidic cell with rough surfaces. Dataset. (LA-UR-21-22267)

In Situ Characterization of Uranium Hydriding Corrosion

Terry Holesinger
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Project Description

Hydride formation / corrosion is a materials problem that affects a broad range of diverse industries that includes manufacturing, transportation, energy and national security. This work focuses on uranium hydride (UH3), which has direct relevance to and is an active research area for laboratory mission for stockpile stewardship. Each step in the hydride formation process contains a number of fundamental unanswered questions – basic gaps in the knowledge that make it currently impossible to predict timing and locations of uranium hydride corrosion on any given surface. Our overall goal is to change this and produce a predictive (theory) and verification (experiment) framework for understanding and directly observing the hydrogen(H) corrosion process in uranium. The pioneering research we propose is to predict and directly observe across all length scales the first early-stage nucleation and growth processes of UH3. This includes identifying the pathways and structural conditions that facilitate hydride formation, no easy task given that the hydride process starts as a subsurface phenomena in technologically applied materials. The results of our work will have an immediate impact on DOE/NNSA missions for stockpile stewardship. Understanding and controlling hydride formation is an important aspect of ensuring material reliability in an aging weapons stockpile.

Publications

Journal Articles

Janish, M. T., M. M. Schneider, E. F. Holby, A. W. Richards, R. K. Schulze and T. G. Holesinger. Hydride mapping in uranium using MLLS fitting of electron energy-loss spectra. Submitted to *Journal of Metals*. (LA-UR-19-32305)

Reports

Holesinger, T. G., J. P. M. Romero, M. R. Middlemas and A. D. Wall. Scanning Electron Microscopy Analysis of Sample MAD-0368-C78. Unpublished report. (LA-CP-20-20414)

Presentation Slides

Holby, E. F. w18_uhydride Scientific Highlight. . (LA-UR-19-21896)

Holby, E. F. Experimental and Modeling work of Sigma Division's Electrochemistry and Corrosion Team. Presented at *Workshop on Corrosion for Mission Science*, Los Alamos, New Mexico, United States, 2021-03-23 - 2021-03-24. (LA-UR-21-22655)

Holby, E. F., M. A. Hill, T. G. Holesinger, M. T. Janish, S. K. Lawrence, A. W. Richards, M. M. Schneider, R. K. Schulze and E. L. Tegtmeier. Uranium Hydride Corrosion: Atomistic Modeling. Presented at *DOE Technical Meeting*, Los Alamos, New Mexico, United States, 2019-06-03 - 2019-06-03. (LA-UR-19-24795)

Holesinger, T. G., M. M. Schneider, M. T. Janish, E. F. Holby, E. L. Tegtmeier, R. K. Schulze and A. W. Richards. New Insights into Early Stage Uranium Hydride Growth. Presented at *MS&T 2019*, Portland, Oregon, United States, 2019-09-29 - 2019-10-03. (LA-UR-19-29767)

Holesinger, T. G., M. M. Schneider, M. T. Janish, E. F. Holby, R. K. Schulze, M. A. Hill, E. L. Tegtmeier, S. K. Lawrence and A. W. Richards. Uranium Hydride Corrosion: Microscopy & in situ Experiments. Presented at *DOE Technical Meeting*, Los Alamos, New Mexico, United States, 2019-06-03 - 2019-06-03. (LA-UR-19-24751)

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, M. A. Hill, E. L. Tegtmeier, S. K. Lawrence, R. K. Schulze and A. W. Richards. Early Stage Uranium Hydride Development in Cast U238. Presented at *Presentation to external agency*, Reading, United Kingdom, 2020-02-12 - 2020-02-14. (LA-UR-20-20934)

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, R. K. Schulze, A. W. Richards, E. L. Tegtmeier, M. J. Aloi and M. A. Hill. In situ Characterization of Uranium Hydriding Corrosion. . (LA-UR-20-23610)

Schneider, M. M. Electron Microscopy of Hydride Actinides. . (LA-UR-19-21935)

Posters

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, R. K. Schulze, E. L. Tegtmeier and A. W. Richards. Towards

Understanding the Atomistic to Mesoscopic Processes in Uranium Hydride Nucleation and Growth. Presented at *Pu Futures - The Science 2018*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28414)

Janish, M. T., M. M. Schneider, T. G. Holesinger, A. W. Richards, E. F. Holby and R. K. Schulze. Mapping Uranium Hydride Corrosion with Electron Energy-Loss Spectroscopy. Presented at *University Workshop on Damage, Shock, and Characterization*, Los Alamos, New Mexico, United States, 2019-07-30 - 2019-08-01. (LA-UR-19-27367)

Chemistry of a New Oxidation State for the Early Transuranic Elements

Andrew Gaunt
20190091ER

Project Description

Extremely rare and specialized radiological capabilities at Los Alamos National Laboratory will be utilized to synthesize compounds in the unusually low +2 oxidation state to conduct fundamental chemical syntheses of the highly radioactive elements of neptunium, plutonium and americium. Chemical control through oxidation state chemistry is a central tenet of actinide separation processes in the nuclear fuel cycle and waste remediation strategies (energy security) - advancement of such control can only be achieved rationally through elucidation of the electronic structure in actinide compounds and understanding the factors that favor particular oxidation states. This fundamental science will be published in top journals, be internationally recognized as world leading and of direct benefit to Department of Energy Office of Science programs to solve basic research needs in their Heavy Element Chemistry program (the 'f-electron' grand challenge). In addition, plutonium science is central to the national security mission of Los Alamos, and any significant new understanding in the chemistry of this element is clearly important.

Publications

Journal Articles

P. Goodwin, C. A., A. W. Schlimgen, T. E. Albrecht-Sch \xc3\xb6nzart, E. R. Batista, A. J. Gaunt, M. T. Janicke, S. A. Kozimor, B. L. Scott, L. M. Stevens, F. D. J. White and P. Yang. Structural and spectroscopic comparison of soft-Se vs hard-O donor bonding in trivalent americium/neodymium molecules. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-21-20831)

P. Goodwin, C. A., J. Su, L. M. Stevens, F. D. J. White, T. E. Albrecht-Schonzart, E. R. Batista, J. N. Cross, W. J. Evans, A. N. Gasier, A. J. Gaunt, M. T. Janicke, T. J. Jenkins, S. A. Kozimor, I. May, B. L. Scott, J. M. Sperling, C. J. Windorff and P. Yang. Bonding and Electronic Structure in a Crystallographically Authenticated Organocalifornium Complex. Submitted to *Nature Chemistry*. (LA-UR-20-28515)

*P. Goodwin, C. A., J. Su, T. E. Albrecht-Schmitt, A. V. Blake, E. R. Batista, S. R. Daly, S. Dehnen, W. J. Evans, A. J. Gaunt, S. A. Kozimor, N. Lichtenberger, B. L. Scott and P. Yang. [Am(C Me H)]: An Organometallic Americium Complex. 2019. *Angewandte Chemie International Edition*. **58** (34): 11695-11699. (LA-UR-19-25159 DOI: 10.1002/anie.201905225)

Staun, S. L., L. M. Stevens, D. E. Smiles, C. A. P. Goodwin, B. S. Billow, B. L. Scott, G. Wu, A. Tondreau, A. J. Gaunt and T. W. Hayton. Expanding the Non-aqueous Chemistry of Neptunium: Synthesis and Structural Characterization of [Np(NR2)3Cl], [Np(NR2)3Cl]1-, and [Np{N(R)(SiMe2CH2)}2(NR2)]1- (R = SiMe3). Submitted to *Inorganic Chemistry*. (LA-UR-21-21036)

Stevens, L. M., R. K. Carlson, A. J. Gaunt, F. D. J. White, C. A. P. Goodwin, T. F. Jenkins, B. L. Scott, E. R. Batista, W. J. Evans, S. A. Kozimor and P. Yang. [NpIICptet3]1-: Deciphering the Role of Ligand Sterics and Electronics on Formation, Stability, and Electronic Structure of [NpIICpR3]1- Complexes. Submitted to *Chemical Communications*. (LA-UR-20-28672)

Reports

P. Goodwin, C. A., J. Su, L. M. Stevens, F. D. J. White, M. T. Janicke, I. May, C. J. Windorff, J. M. Sperling, A. N. Gaiser, J. N. Cross, T. E. Albrecht-Schmitt, T. F. Jenkins, E. R. Batista, W. J. Evans, A. J. Gaunt, S. A. Kozimor, B. L. Scott and P. Yang. Bonding and Electronic Structure in a Crystallographically Authenticated Organocalifornium Complex. Unpublished report. (LA-UR-19-32441)

Presentation Slides

P. Goodwin, C. A. Np and Cf(III) Cp organometallic complexes. . (LA-UR-19-20947)

P. Goodwin, C. A. Cyclic voltammetry data (C23) on [Pu(tBuPyNO)4], a Pu(IV) coordination complex with a nitroxide ligand. . (LA-UR-19-21962)

P. Goodwin, C. A. f-element Chemistry: Oxidation States, Bonding, and Electronic Structures. . (LA-UR-19-20861)

Murillo, J., C. A. P. Goodwin, L. M. Stevens, A. J. Gaunt and S. Fortier. Murillo data. . (LA-UR-21-22354)

Stevens, L. M. Elucidation of Electronic Structure and Bonding in Organometallic Actinide Complexes. . (LA-UR-20-23302)

Stevens, L. M. and A. J. Gaunt. Photos. . (LA-UR-20-22798)

Posters

Stevens, L. M., C. A. P. Goodwin, W. J. Evans, S. A. Kozimor and A. J. Gaunt. Probing Electronic Structure of Organometallic Transuranic Complexes. . (LA-UR-19-28587)

Understanding and Predicting Hydrocarbon Behaviors in Nanopores of Tight Reservoirs

Qinjun Kang
20190153ER

Project Description

Energy security and national security are inherently linked. National security can be either strengthened or weakened through energy security. That is why energy security is a central issue of interest to the Laboratory, Department of Energy(DOE)/National Nuclear Security Administration(NNSA), and the nation. This research directly supports DOE/NNSA's energy security/ independence goal by addressing the fundamental problems underlying the low recovery rates of tight oil/gas productions. The knowledge and fundamental understanding gained from this research may provide important insights for designing better production strategies to maximize recovery rates from the reservoir matrix, paving the way towards U.S. independence of foreign petroleum resources in the foreseeable future while minimizing the environmental impact. The advanced experimental and modeling capabilities to be developed in this project will also be applicable to other mission-critical areas such as carbon dioxide (CO2) sequestration and enhanced geothermal systems.

Publications

Journal Articles

*Bakhshian, S., M. Murakami, S. A. Hosseini and Q. Kang. Scaling of Imbibition Front Dynamics in Heterogeneous Porous Media. 2020. *Geophysical Research Letters*. **47** (14): e2020GL087914. (LA-UR-20-22139 DOI: 10.1029/2020GL087914)

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*Feifei, Q., A. Mazloomi Moqaddam, L. Del Carro, K. Qinjun, T. Brunschwiler, D. Derome and J. Carmeliet. Tricoupled hybrid lattice Boltzmann model for nonisothermal drying of colloidal suspensions in micropore structures. 2019. *Physical Review E*. **99** (5): 053306. (LA-UR-19-22956 DOI: 10.1103/PhysRevE.99.053306)

Gong, Y., M. Z. S. Mehana, I. El-monier and H. S. Viswanathan. Proppant Placement in Complex Fracture Geometries: A Computational Fluid Dynamics. Submitted to *Scientific Reports*. (LA-UR-19-29884)

Gong, Y., M. Z. S. Mehana and I. El-monier. Proppant Placement in Complex Fracture Geometries: a Coupled CFD-DEM Approach. Submitted to *Journal of Natural Gas Science and Engineering*. (LA-UR-20-26091)

Guiltinan, E. J., J. E. Santos, B. M. Cardenas, N. D. Espinoza and Q. Kang. Two-Phase Fluid Flow Properties of Rough Fractures With Heterogeneous Wettability: Analysis With Lattice Boltzmann Simulations. 2021. *Water Resources Research*. **57** (1): e2020WR027943. (LA-UR-20-23393 DOI: 10.1029/2020WR027943)

Lee, S., H. Xu, J. Wempner, H. Xu and J. Wen. Gold nanoparticles in Marcellus Shale. Submitted to *Nature Communications*. (LA-UR-19-26399)

*Lubbers, N., A. Agarwal, Y. Chen, S. Son, M. Mehana, Q. Kang, S. Karra, C. Junghans, T. C. Germann and H. S. Viswanathan. Modeling and scale-bridging using machine learning: nanoconfinement effects in porous media. 2020. *Scientific Reports*. **10** (1): 13312. (LA-UR-20-22679 DOI: 10.1038/s41598-020-69661-0)

S. Mehana, M. Z., E. J. Guiltinan, V. V. Vesselinov, J. D. Hyman, R. S. Middleton, Q. Kang and H. S. Viswanathan. Machine-learning predictions of the shale wells' performance. 2021. *Journal of Natural Gas Science and Engineering*. **88**: 103819. (LA-UR-20-23394 DOI: 10.1016/ j.jngse.2021.103819)

S. Mehana, M. Z., S. Hosseini, T. A. Meckel and H. S. Viswanathan. Modelling the Carbon Dioxide Plume Using Modified-Invasion-Percolation Simulation. Submitted to *Transport in Porous Media*. (LA-UR-19-26910)

S. Mehana, M. Z. and J. Callard. Complex Fracture Depletion Model for Reserves Estimations in Shale. Submitted to *journal of energy resources technology*. (LA-UR-20-21346)

S. Mehana, M. Z. and M. Fahes. The Impact of the Geochemical Interactions on the Fate of Fracturing Fluid and Well Performance in Shale Reservoirs.. Submitted to *Petroleum*. (LA-UR-20-20809)

Mohamed, T., M. Z. S. Mehana and Z. Reza. Coalbed methane Review and Outlook. Submitted to *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*. (LA-UR-20-21924)

Neil, C. W., M. Z. S. Mehana, R. P. J. Hjelm, M. E. Hawley, E. B. Watkins, Y. Mao, H. S. Viswanathan, Q. Kang and H. Xu. Pore size dependence of pressure cycling and nanopore confinement effects on methane recovery from a shale matrix. Submitted to *Nature Communications*. (LA-UR-20-22897)

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*Neil, C. W., R. P. Hjelm, M. E. Hawley, E. B. Watkins, C. Cockreham, D. Wu, Y. Mao, T. B. Fischer, M. R. Stokes and H. Xu. Small-angle Neutron Scattering (SANS) Characterization of Clay- and Carbonate-rich Shale at Elevated Pressures. 2020. *Energy & Fuels*. **34** (7): 8178-8185. (LA-UR-19-30857 DOI: 10.1021/acs.energyfuels.0c01009)

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Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, J. Carmeliet and D. Derome. Three influential factors on colloidal nanoparticle deposition for heat conduction enhancement in 3D chip stacks. 2021. *Applied Thermal Engineering*. 116585. (LA-UR-20-23176 DOI: 10.1016/j.applthermaleng.2021.116585)

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Wang, H., L. Chen, Z. Qu, Y. Yin, Q. Kang, B. Yu and W. Q. Tao. Modeling of multi-scale transport phenomena in shale gas production — A critical perspective. Submitted to *Applied Energy*. (LA-UR-19-27980)

*Zhao, B., C. W. MacMinn, B. K. Primkulov, Y. Chen, A. J. Valocchi, J. Zhao, Q. Kang, K. Bruning, J. E. McClure, C. T. Miller, A. Fakhari, D. Bolster, T. Hiller, M. Brinkmann, L. Cueto-Felgueroso, D. A. Cogswell, R. Verma, M. Prodanovic, J. Maes, S. Geiger, M. Vassvik, A. Hansen, E. Segre, R. Holtzman, Z. Yang, C. Yuan, B. Chareyre and R. Juanes. Comprehensive comparison of pore-scale models for multiphase flow in porous media. 2019. *Proceedings of the National Academy of Sciences*. **116** (28): 13799-13806. (LA-UR-19-21742 DOI: 10.1073/pnas.1901619116)

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, D. Derome and J. Carmeliet. Pore-scale simulation of drying in porous media using a hybrid lattice Boltzmann - pore network model. Submitted to *Drying Technology*. (LA-UR-21-20066)

*Zhao, J., Q. Kang, Y. Wang, J. Yao, L. Zhang and Y. Yang. Viscous Dissipation and Apparent Permeability of Gas Flow in Nanoporous Media. 2020. *Journal of Geophysical Research: Solid Earth*. **125** (2): e2019JB018667. (LA-UR-19-30105 DOI: 10.1029/2019JB018667)

Conference Papers

Guiltinan, E. J., J. Santos and Q. Kang. Residual Saturation During Multiphase Displacement in Heterogeneous Fractures with Novel Deep Learning Prediction. Presented at *Unconventional Resources Technology Conference (URTeC)*. (Austin, Texas, United States, 2020-07-20 - 2020-07-22). (LA-UR-20-24072)

Presentation Slides

Chen, Y., Q. Kang, H. S. Viswanathan and A. J. Valocchi. Investigation of the inertial effects during the drainage process in a real rock. Presented at *InterPore 11th Annual Meeting*, Valencia, Spain, 2019-05-06 - 2019-05-10. (LA-UR-19-24097)

Guiltinan, E. J. Seminar at Southwest Research Institute. . (LA-UR-20-27283)

Guiltinan, E. J., J. E. Santos and Q. Kang. Residual Saturation During Multiphase Displacement in Heterogeneous Fractures with Novel Deep Learning Prediction. Presented at *Unconventional Resources Technology Conference*, Austin, Texas, United States, 2020-07-20 - 2020-07-22. (LA-UR-20-24898)

Kang, Q. Pore-Scale Direct Numerical Simulation of Transport and Interfacial Phenomena. . (LA-UR-18-29213)

Kang, Q. 2018 Annual Report of Institutional Computing Project w17_porescale: Figures. . (LA-UR-19-21741)

Kang, Q. Pore-Scale Direct Numerical Simulation of Flow and Transport in Porous Media. . (LA-UR-20-25563)

Kang, Q. Pore-Scale Direct Numerical Simulation of Flow and Transport in Porous Media. Presented at *InterPore 12th Annual Meeting*, Los Alamos, New Mexico, United States, 2020-08-31 - 2020-08-31. (LA-UR-20-26798)

Kang, Q. Progress Report of Institutional Computing Project w20_porousmedia: Figures. . (LA-UR-21-21833)

Kang, Q., M. Z. S. Mehana, H. Xu and T. P. Nguyen. Understanding and Predicting Hydrocarbon Behaviors in Nanopores of Tight Reservoirs. Presented at *TAMU visit*, college station, Texas, United States, 2019-11-25 - 2019-11-26. (LA-UR-19-31750)

S. Mehana, M. Z. Modeling Subsurface Phenomena. . (LA-UR-20-28542)

S. Mehana, M. Z. Molecular modeling of subsurface phenomena. Presented at *Invited talk to Sandia geochemistry team*, ABQ, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-21309)

Nguyen, T. P. Using Methane Isotope Signatures to Evaluate and Improve the Shale Production Curve. Presented at *CSES Symposium*, Los Alamos, New Mexico, United States, 2019-08-15 - 2019-08-15. (LA-UR-19-30282)

Posters

S. Mehana, M. Z., Q. Kang and H. S. Viswanathan. Molecular Modeling of the Fluid Behavior in shale Nanopores. Presented at *Postdoc Research Symposium*, Los alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28653)

Neil, C. W., R. P. J. Hjelm, E. B. Watkins, M. E. Hawley, Y. Mao, T. Fischer, M. Stokes, M. Z. S. Mehana, H. S. Viswanathan, Q. Kang and H. Xu. Probing Fluid Behavior in Shale Nanopores with High-Pressure Small-Angle Neutron Scattering. Presented at *CNES Capability Review Virtual meeting*, Los Alamos, New Mexico, United States, 2020-09-14 - 2020-09-14. (LA-UR-20-26381)

Using Solar Energetic Protons to Monitor the Outer Magnetosphere

Steven Morley
20190262ER

Project Description

This project targets understanding and modeling of the outer reaches of Earth's magnetic field, with a specific goal of specifying and predicting the access of solar energetic particles within Earth's magnetic field. This magnetic field plays a critical role in protecting assets such as the International Space Station, satellites, and aircraft from harmful radiation. As this part of Earth's magnetic field is sparsely measured we expect to develop new understanding of how the Sun drives space weather, as well as underpinning a new capability that can improve satellite and aviation safety during space weather events with predictive capabailites.

Publications

Journal Articles

*Chakraborty, S. and S. K. Morley. Probabilistic prediction of geomagnetic storms and the Kp index. *Journal of Space Weather and Space Climate*. **10**: 36. (LA-UR-20-20109 DOI: 10.1051/swsc/2020037)

*Chen, Y., S. K. Morley and M. R. Carver. Global Prompt Proton Sensor Network: Monitoring Solar Energetic Protons Based on GPS Satellite Constellation. 2020. *Journal of Geophysical Research: Space Physics*. **125** (3): e2019JA027679. (LA-UR-19-31569 DOI: 10.1029/2019JA027679)

Engel, M. A., Z. Li, M. Hudson, B. Kress, M. Patel, M. Qin and R. Selesnick. Solar Energetic Proton Access to the Inner Magnetosphere during the 7-8 September 2017 event. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-21-20075)

*Morley, S. K. Challenges and Opportunities in Magnetospheric Space Weather Prediction. 2020. *Space Weather*. **18** (3). (LA-UR-19-26681 DOI: 10.1029/2018SW002108)

Olifer, L., I. R. Mann, L. G. Ozeke, S. K. Morley and H. L. Louis. On the Formation of Phantom Electron Phase Space Density Peaks in Single Spacecraft Radiation Belt Data. Submitted to *Geophysical Research Letters*. (LA-UR-21-22136)

*Qin, M., M. Hudson, B. Kress, R. Selesnick, M. Engel, Z. Li and X. Shen. Investigation of Solar Proton Access Into the Inner Magnetosphere on 11 September 2017. 2019. *Journal of Geophysical Research: Space Physics*. **124** (5): 3402-3409. (LA-UR-18-31475 DOI: 10.1029/2018JA026380)

Smirnov, A. G., M. Berrendorf, Y. Y. Shprits, E. A. Kronberg, H. J. Allison, N. A. Aseev, I. S. Zhelavskaya, S. K. Morley, F. Effenberger and R. Vasile. Medium Energy Electron Flux in Earth's Outer Radiation Belt (MERLIN): A Machine Learning Model. Submitted to *Space Weather*. (LA-UR-20-22970)

Thompson, R. L., S. K. Morley, C. E. Watt, S. N. Bentley and P. D. Williams. Pro-L* - A probabilistic L* mapping tool for ground observations to the magnetic equator. Submitted to *Space Weather*. (LA-UR-20-25802)

Conference Papers

Chen, Y., M. R. Carver, S. K. Morley and A. S. Hoover. Determining Ionizing Doses in Medium Earth Orbits Using Long-Term GPS Particle Measurements. Presented at *IEEE Aerospace Conference 2021*. (Big Sky, Montana, United States, 2021-03-06 - 2021-03-13). (LA-UR-20-28033)

Reports

Morley, S. K. Institutional Computing Annual Report. Unpublished report. (LA-UR-20-26358)

Thompson, R. L. and S. K. Morley. Pro-L*: probabilistic hourly L* values, with associated McIlwain Lm, magnetic field intensity B, and Cartesian coordinates for 7 global magnetic field models in the Northern Hemisphere in the period 2006-2016. Unpublished report. (LA-UR-19-29115)

Presentation Slides

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Chen, Y., S. K. Morley, M. R. Robert and A. S. Hoover. Understanding Solar Energetic Proton Effects in Space and Ground-level from GPS-based Measurements. Presented at *AGU Fall meeting 2020*, Los Alamos, New Mexico, United States, 2020-11-01 - 2020-11-01. (LA-UR-20-29472)

Jordanova, V. K., S. K. Morley, E. H. Lay and R. A. Haaser. Investigations of Magnetosphere-Ionosphere Coupling During the September 2017 Storm. Presented at *2020 Virtual GEM Summer Workshop*, Santa Fe, New Mexico, United States, 2020-07-20 - 2020-07-23. (LA-UR-20-25224)

Morley, S. K. Statistical Modeling and Machine Learning for Space Physics. Presented at *Coupling, Energetics and Dynamics of Atmospheric Regions (CEDAR) workshop*, Santa Fe, New Mexico, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25471)

Morley, S. K. Physics-Based Modeling of Space Weather During Large and Extreme Geomagnetic Storms. . (LA-UR-20-26360)

Morley, S. K., J. R. Woodroffe, D. T. Welling, G. S. Bowers, M. R. Carver, A. L. Stricklan and Y. Chen. Combining particle tracing and constellation energetic particle data. Presented at *Workshop on machine Learning, data Mining and data Assimilation in Geospace (LMAG2020)*, Online, Maryland, United States, 2020-09-22 - 2020-09-22. (LA-UR-20-27398)

Posters

Carver, M. R., Y. Chen and S. K. Morley. The GPS Constellation of Satellites as a Global Proton Sensor Netowrk. Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-20-20580)

Chakraborty, S. and S. K. Morley. Probabilistic Geomagnetic Storm Forecasting Using Machine Learning. Presented at *Coupling, Energetics and Dynamics of Atmospheric Regions (CEDAR) Workshop*, Santa Fe, New Mexico, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25470)

Morley, S. K., J. R. Woodroffe, M. R. Carver, Y. Chen, A. L. Stricklan, D. T. Welling, J. Haiducek and G. S. Bowers. Improving Predictions of Solar Energetic Particle Access at Medium Earth Orbit. Presented at *American Meteorological Society 101st Annual Meeting*, Online, California, United States, 2021-01-10 - 2021-01-15. (LA-UR-21-20077)

Morley, S. K., M. R. Carver, Y. Chen and A. L. Stricklan. GPS: A Constellation Mission Measuring Solar Energetic Protons and the Electron Radiation Belts. Presented at *American Meteorological Society 100th Annual Meeting*, Boston, Massachusetts, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20317)

Innovating Wildfire Representation in Earth System Models (ESMs)

Alexandra Jonko
20190310ER

Project Description

Changes in local and regional climate will have a significant impact on critical infrastructure and have been recognized as a national security concern, which the Department of Energy is working to address through its Energy Exascale Earth System Model (E3SM) project. Wildland fire is an important climate process which interacts with ecosystems and the atmosphere through two-way feedbacks. However, it is currently represented crudely in Earth System Models - including E3SM -, which neglect the impacts of local topography and vegetation on wildland fire behavior. These shortcomings impede our ability to accurately simulate important interactions between fire and climate, and ultimately limit our ability to make predictions about future climate impacts on ecosystems and critical infrastructure, as well as water, carbon, and energy budgets. Our project proposes to improve the representation of wildland fire activity within Earth System Models and to enable them to accurately capture fire-climate feedbacks. Our novel, multi-scale model-based approach will reduce uncertainty in climate projections, directly supporting decision-making for national security applications related to the environment and infrastructure.

Publications

Journal Articles

Jonko, A., K. Yedinak, R. R. Linn and J. L. Conley. Sensitivity of grass fires burning in marginal conditions to small perturbations in the turbulent wind field. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-20-23811)

Linn, R. R. Quick Study Fluid Dynamics of Wildfire. Submitted to *Physics Today*. (LA-UR-19-30531)

Linn, R. R., J. W. White, J. Furman, B. Williams, K. Hiers, A. Jonko, J. O'Brien, K. Yedinak and S. Goodrick. Modeling Low Intensity Fires: Lessons Learned from 2012 RxCADRE. Submitted to *MDPI Atmosphere*. (LA-UR-20-29541)

*Linn, R. R., S. L. Goodrick, S. Brambilla, M. J. Brown, R. S. Middleton, J. J. O'Brien and J. K. Hiers. QUIC-fire: A fast-running simulation tool for prescribed fire planning. 2020. *Environmental Modelling & Software*. **125**: 104616. (LA-UR-19-27513 DOI: 10.1016/j.envsoft.2019.104616)

Presentation Slides

Jonko, A. Using Supercomputers to Understand Wildfire Behavior. . (LA-UR-19-20192)

Jonko, A. Probabilistic Topography Project Update 5/20. . (LA-UR-20-23810)

Jonko, A., K. E. Bennett, R. R. Linn, J. A. Oliveto and D. R. Livingston. Incorporating effects of topography and subgrid-scale vegetation heterogeneity on fire spread into Earth System Models. Presented at *"California Ecosystem Futures" UC Lab Fees Project Meeting*, Los Alamos, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-21308)

Jonko, A., K. E. Bennett, R. R. Linn, S. Brambilla and D. R. Livingston. Incorporating effects of small-scale topography and vegetation heterogeneity on Wildland fire in Earth System Models. Presented at *AFE Fire Congress*, Tucson, Arizona, United States, 2019-11-18 - 2019-11-22. (LA-UR-19-31623)

Jonko, A., K. Yedinak, J. Conley, R. R. Linn, A. L. Atchley and R. Parsons. Sensitivity of modeled fire behavior to small perturbations in initial conditions. . (LA-UR-21-20605)

Jonko, A., K. Yedinak, R. R. Linn, J. L. Conley, R. Parsons and A. L. Atchley. Sensitivity of modeled fire behavior to small perturbations in initial conditions. Presented at *6th International Wildland Fore Behavior and Fuels Conference*, Albuquerque, New Mexico, United States, 2019-04-29 - 2019-05-02. (LA-UR-19-23934)

Jonko, A., R. R. Linn and K. E. Bennett. Innovating Wildfire Representation in ESMs. Presented at *Meeting with potential collaborators at NCAR*, Boulder, Colorado, United States, 2018-10-17 - 2018-10-18. (LA-UR-18-29850)

Jonko, A. and J. A. Oliveto. Check-in with Neda Yaghoobian (FSU). . (LA-UR-20-24416)

Linn, R. R. Institutional Computing Report slide for FIRETEC project. . (LA-UR-19-22597)

Linn, R. R. Modeling the dynamical coupling between fires and atmospheric hydrodynamics. . (LA-UR-19-30397)

Linn, R. R. Process-based fire/atmosphere modeling: opportunities and challenges. Presented at *NIST: Large Outdoor Fire Modeling Workshop*, Gaithersberg, Maryland, United States, 2019-03-18 - 2019-03-18. (LA-UR-19-22599)

Linn, R. R., A. Jonko, J. W. White, I. M. Runde, C. Sieg and R. Parsons. Coupled Fire-Atmosphere Interactions controlling the combined influences of wind and slope fire behavior. Presented at *International Fire Behavior and Fuels Conference*, Albuquerque, New Mexico, United States, 2019-04-29 - 2019-04-29. (LA-UR-19-23931)

Linn, R. R., I. Altintas, J. K. Hiers, R. S. Middleton and V. V. Vesselinov. AI and Wildland Fire – Needs / Opportunities. Presented at *SAGE workshop*, Chicago, Illinois, United States, 2020-05-12 - 2020-05-12. (LA-UR-20-23559)

Linn, R. R., S. Goodrick, E. Koo, A. Jonko, C. Seig, M. J. Brown and S. Brambilla. Physics-Based Fire/Atmosphere Modeling: Opportunities and Challenges. Presented at *National Academy of Sciences Workshop on Wildfire Modeling*, Berkeley, New Mexico, United States, 2019-10-07 - 2019-10-07. (LA-UR-19-30396)

Oliveto, J. A. Effects of Sub-Grid Topography in Earth System Model Representation of Wildfires. . (LA-UR-20-26551)

Oliveto, J. A. Probablistic Topography Neda Check-in 10/21. . (LA-UR-20-28541)

Oliveto, J. A. Correcting Area Burned in Earth System Models Using a Probabilistic Representation of Sub-Grid Topography (AGU Poster 2020). Presented at *American Geophyical Union Meeting Fall 2020*, Los Alamos (Online), New Mexico, United States, 2020-12-07 - 2020-12-07. (LA-UR-20-29442)

Oliveto, J. A. Influence of topography and vegetation heterogeneity on wildfire in Earth System Models. . (LA-UR-21-22061)

Illuminating Plutonium: Spectroelectrochemisty in High Temperature Molten Salts

Benjamin Stein
20190364ER

Project Description

The production of plutonium "pits" for nuclear weapons requires very high-purity (>99.9% pure) plutonium metal. The only current source of this high-purity metal is the electrorefining process, which utilizes a high-temperature (~900C) molten salt bath. While this process produces the necessary purity, the recovery of valuable plutonium needs improvement and the refining time is very long. Little is known about the behavior of plutonium in these extreme environments, making it difficult to suggest rational improvements to the electrorefining process. We will develop a capability designed to monitor the chemistry of plutonium in real time as a function of process changes using a variety of optical and X-ray based techniques. This will give us a more complete understanding of these systems, allowing us to inform our plutonium processing colleagues about potential process improvements.

Publications

Reports

Stein, B. and N. H. Lam. Total Moisture Analysis of Salts by Dissolution. Unpublished report. (LA-UR-21-22658)

Presentation Slides

Stein, B., Z. R. Jones, P. Yang, E. R. Batista, S. K. Schrell, F. Rein Rocha, N. H. Anderson and V. Mocko. Plutonium speciation in molten salts. Presented at *JOWOG 22*, Los Alamos, New Mexico, United States, 2019-07-15 - 2019-07-15. (LA-UR-19-27622)

Biogenic Uranium Isotope Fractionation for Biotechnology

Robert Williams
20190372ER

Project Description

Since the discovery of Uranium (U), it has received a great deal of attention from scientists and governments worldwide, largely due to its fissile properties. The complex biological processes that allow microorganisms to sequester and chemically alter actinides is of great importance for environmental and biosecurity applications. We will assess the practicality of microbial-based or microbial-inspired biotechnology systems for uranium isotope fractionation, by understanding how organisms process the uranium isotopes and favor the formation of insoluble uranium oxide. We will utilize the Laboratory's cross-cutting expertise in biochemistry, microbiology and actinide chemistry to elucidate the mechanism of uranium isotope fractionation that occurs during bioreduction. We will focus on the characterization of the three main aspects of uranyl bioreduction that likely control U isotope fractionation; U adsorption, sequestration, and/or uptake and its subsequent reduction; cellular processes that support the electron transport pathways and enzymatic reduction of uranium; and characterizing/ mapping of the cellular location of U reduction and precipitation. Ultimately, we will evaluate the practicality for biotechnology applications of the mechanistic driver(s) of U fractionation and the processes from the interactions between the cell and soluble U that lead to the accumulation of U mineral precipitates near or within the cell.

Publications

Journal Articles

*Jemison, N. E., M. T. Bizjack, T. M. Johnson and J. L. Druhan. Influence of physical and chemical hydrology on bioremediation of a U-contaminated aquifer informed by reactive transport modeling incorporating 238U/235U ratios. 2020. *Geochimica et Cosmochimica Acta*. **269**: 303-328. (LA-UR-19-21464 DOI: 10.1016/j.gca.2019.10.031)

*Jemison, N., P. Reimus, R. Harris, H. Boukhalfa, J. Clay and K. Chamberlain. Reduction and potential remediation of U(VI) by dithionite at an in-situ recovery mine: Insights gained by \xce\xb4238U. 2020. *Applied Geochemistry*. **115**: 104560. (LA-UR-19-27182 DOI: 10.1016/j.apgeochem.2020.104560)

Lefebvre, P., V. Noel, K. V. Lau, N. E. Jemison, K. L. Weaver, K. H. Williams and K. Maher. Isotopic Fingerprint of Uranium Accumulation and Redox Cycling in Floodplains of the Upper Colorado River Basin. 2019. *Environmental Science & Technology*. acs.est.8b05593. (LA-UR-19-20457 DOI: 10.1021/acs.est.8b05593)

Reports

Miner, J. C. Institutional Computing Report (w19_foldamers). Unpublished report. (LA-UR-20-23820)

Miner, J. C., H. T. B. Nguyen and P. W. Peterson. Characterizing neurotoxicology and CNS therapeutics through molecular modeling (IC Proposal). Unpublished report. (LA-UR-20-26930)

Presentation Slides

Guardincerri, E. Colloquium at Drexel University about Muon Radiography at the Los Alamos National Laboratory. . (LA-UR-19-20983)

Kolade, B. A., J. C. Miner and R. F. Williams. Validating Experimental Results of Cardiac Glycosides and Monoterpene Indole Alkaloids using Cheminformatics. Presented at *Biophysical Society Meeting*, Boston, Massachusetts, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-20513)

Marti-Arbona, R., N. Jemison, R. F. Williams, H. Boukhalfa, C. M. Yeager, N. Xu and V. V. Vesselinov. Biogenic uranium isotope fractionation. . (LA-UR-20-23926)

Miner, J. C. Quantifying interactions of biomolecules and cosolvents - or - linking structure to solution. . (LA-UR-19-24546)

Miner, J. C. Monitoring microgravity effects on biomolecules. Presented at *Center for Space and Earth Science CSES SRR Microgravity Symposium*, Los Alamos, New Mexico, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28536)

Posters

Jemison, N. E., H. Boukhalfa, R. Marti-Arbona, C. M. Yeager and N. Xu. Mechanisms of Uranium Isotope Fractionation. Presented at *Goldschmidt 2019*, Barcelona, Spain, 2019-08-18 - 2019-08-23. (LA-UR-19-27953)

Understanding Glycan Dynamics and Heterogeneity for Effective Human Immunodeficiency Virus (HIV) Vaccine Development

Kshitij Wagh
20190441ER

Project Description

Our long-term goal is to better understand the important role of protein-attached sugars (“glycans”) in infectious disease, immunology, cancer, and other biological fields, and to apply this knowledge for discovery/design of novel vaccines and therapeutics, and biothreat detection and mitigation. The research proposed here encompasses the development of computational strategies required for realizing our long-term research program, and their application to understanding the role of Human Immunodeficiency Virus (HIV) glycans in successful antibody responses. If successful, this work will directly contribute to the design of effective HIV vaccines designed to elicit broad efficacious antibody responses. Furthermore, our glycan modeling strategies can be applied to different biological fields to extract basic biological data on glycans that are inaccessible to experimental measurement, or are difficult to measure, thereby facilitating high-throughput studies investigating biological importance of glycans. This research directly supports the basic science efforts of the Department of Energy Office of Science Biological and Environmental Research to understand structure and function of complex, biological systems using computational approaches. Our general modeling framework can also be applied to understand other biological phenomena of interest to the DOE/National Nuclear Security Administration such as plant sugars, algal biofuels, etc.

Publications

Journal Articles

Lopez Bautista, C. A., K. Wagh, S. Chakraborty and S. Gnanakaran. Parametrization of reductive models for N-glycans: A case study of the HIV-1 Env glycoprotein dynamics. Submitted to *Glycobiology*. (LA-UR-20-26658)

Shen, X., H. Tang, C. McDanal, K. Wagh, W. M. Fischer, J. P. Theiler, H. Yoon, B. F. Haynes, K. O. Saunders, S. Gnanakaran, N. W. Hengartner, R. Pajon, G. Smith, G. Glenn, B. T. M. Korber and D. C. Montefiori. SARS-CoV-2 variant B.1.1.7 is susceptible to neutralizing antibodies elicited by ancestral Spike vaccines. 2021. *Cell Host & Microbe*. (LA-UR-21-20697 DOI: 10.1016/j.chom.2021.03.002)

Wagh, K., B. H. Hahn and B. T. M. Korber. Hitting the sweet spot: exploiting HIV-1 glycan shield for induction of broadly neutralizing antibodies. Submitted to *Current Opinion in HIV and AIDS*. (LA-UR-20-26631)

Presentation Slides

Lopez Bautista, C. A. Capability allows faster screening of HIV Env with native glycan diversity. . (LA-UR-20-21204)

Lopez Bautista, C. A. Large scale MD to predict Epitope regions in HIV Env. . (LA-UR-21-21427)

Passive MemComputing in Lithographic Arrays of Interacting Magnetic Nanoislands

Francesco Caravelli
20200105ER

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.

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., M. D. Saccone and C. Nisoli. On the Degeneracy of Spin Ice Graphs, and Its Estimate via the Bethe Permanent. Submitted to *Proceedings of the Royal Society A. Mathematical, Physical and Engineering Sciences*. (LA-UR-21-20434)

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. B. Saxena and J. V. Selinger. Control of liquid crystal skyrmions towards designing re-configurable materials. Submitted to *Physical Review Letters, arxiv.org*. (LA-UR-20-20733)

King, A., C. Nisoli and A. Lopez-Bezanilla. Qubits Spin Ice. Submitted to *Science*. (LA-UR-20-30163)

May, A., M. D. Saccone, A. M. Van Den Berg, J. Askey, M. Hunt and S. Ladak. Magnetic Charge Propagation upon a 3D Artificial Spin-ice. Submitted to *Nature Communications*. (LA-UR-21-22700)

Merrigan, C., Y. Shokef and C. Nisoli. Topological Memory and Hysteresis in Ice-like Mechanical Metamaterials. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-28310)

Pisanty, B., E. Oguz, C. Nisoli and Y. Shokef. Topological defects steer stresses in two- and three-dimensional combinatorial mechanical metamaterials. Submitted to *Physical Review Letters*. (LA-UR-20-28535)

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)

Sheldon, F. C., F. Caravelli and A. Kolchinsky. The Computational Capacity of Memristor Reservoirs. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-26991)

Presentation Slides

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

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

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)

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

Scott Hennelly
20200111ER

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.

The Genetic Patterns of Migration in Global Pandemics

Andrey Lokhov
20200121ER

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.

Publications

Journal Articles

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)

Hengartner, N. W., I. Torres, E. Romero-Severson, R. Mahesh, N. R. Ortega, R. Ke and L. Cuellar-Hengartner. Assessing the Impact of Human Mobility to Predict Regional Excess Death in Ecuador. Submitted to *United Nation Development Program Report*. (LA-UR-21-21098)

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., N. W. Hengartner, G. D. Meadors and R. Ke. DECLINE IN GLOBAL TRANSMISSION RATES OFCOVID-19 THROUGH APRIL 16 2020. Submitted to *PLOS One*. (LA-UR-20-23673)

Snyder, J., A. V. Zlotnik and A. Lokhov. Data-driven Selection of Coarse-Grained Models of Coupled Oscillators. Submitted to *Physical Review Research*. (LA-UR-20-27371)

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)

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)

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)

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

Peter Goodwin
20200161ER

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.

Publications

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)

An Actinium-225/Bismuth-213 Generator Based on Millifluidics Controlled Electrodeposition for Radiopharmaceutical Applications

Michael Fassbender
20200165ER

Project Description

Radiopharmaceutical generators are widely used in modern medicine. Radioisotopes provide both diagnostic tools (e.g. Positron Emitting Tomography) and therapeutic treatments for cancer and other diseases. In the US, millions of doses are given per year. These generators work by exploiting chemical differences in a parent/daughter isotope relationship, and a longer-lived parent isotope, such as Actinium-225, serves as a source of a clinically useful shorter-lived daughter, such as Bismuth-213. Targeted Alpha Therapy is an emerging field for the treatment of cancer and other diseases. Alpha emitting radionuclides are attached to disease targeting antibodies and deliver a lethal dose of alpha radiation to targeted cells within ~10 cell lengths. This results in a treatment with minimal impact on healthy tissue. Clinical trials of Actinium-225/Bismuth-213 show great promise for saving 1000s of lives per year.

Publications

Posters

O'Donnell, E. J., G. A. Andrade and A. N. Marchi. 3-D Printing Chemically Resistant Polymers for Millifluidic Chemical Processing Devices. Presented at *LANL Engineer Week*, Los Alamos, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21403)

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

John Dunbar
20200252ER

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.

Publications

Journal Articles

Shakya, M., J. Martí-Carreras and B. Busby. NCBI's Virus Discovery Codeathon: Building the "FIVE" -- Federated Index of Viral Experiments API database. Submitted to *Viruses*. (LA-UR-20-23300)

Engineering green factories for the production of renewable chemicals

Taraka Dale
20200274ER

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.

Inverse Problem Approach to Spacecraft Charging Simulations

Gian Delzanno
20200276ER

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.

Publications

Journal Articles

Borovsky, J. E., G. L. Delzanno, J. A. Valdivia, P. Moya, M. Stepanova, J. Birn, L. W. Blum, W. Lotko and M. Hesse. Outstanding questions in magnetospheric plasma physics: The pollenzo view. 2020. *Journal of Atmospheric and Solar-Terrestrial Physics*. **208**: 105377. (LA-UR-20-22829 DOI: 10.1016/j.jastp.2020.105377)

Delzanno, G. L., J. E. Borovsky, M. G. Henderson, P. A. Resendiz Lira, V. Roytershteyn and D. T. Welling. The impact of cold electrons and cold ions in magnetospheric physics. Submitted to *Journal of Atmospheric and Solar-Terrestrial Physics*. (LA-UR-20-28089)

Presentation Slides

Delzanno, G. L. Spacecraft-charging events from RBSP. . (LA-UR-20-22881)

Delzanno, G. L. Inverse Problem Approach to Spacecraft Charging Simulations. . (LA-UR-20-29809)

Delzanno, G. L., N. Buzulukova, B. Giles, R. Varney and J. E. Borovsky. The impact of the cold plasma in magnetospheric physics. Presented at *VGEM meeting*, Honolulu, Hawaii, United States, 2020-07-21 - 2020-07-21. (LA-UR-20-25535)

Resendiz Lira, P. A., G. L. Delzanno and J. E. Borovsky. Modeling of Cold-Electron Measurements. Presented at *Mini-GEM workshop*, Los Alamos, New Mexico, United States, 2021-01-20 - 2021-01-20. (LA-UR-21-20466)

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

Resendiz Lira, P. A., H. C. Godinez Vazquez, G. L. Delzanno, M. G. Henderson, D. Svyatsky and B. E. Wohlberg. Inverse Problem Approach to Spacecraft Charging Simulations. Presented at *AGU Fall Meeting 2020*, San Francisco, California, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29639)

Godinez Vazquez, H. C., B. E. Wohlberg, P. A. Resendiz Lira and G. L. Delzanno. Estimating Material and Environmental Parameters for Spacecraft Charging using Van Allen Probes Data. Presented at *AGU Fall Meeting 2020*, Los Alamos, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29689)

Nanotherapeutic Adjuvants for Sepsis

Jessica Kubicek-Sutherland
20200300ER

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.

Publications

Journal Articles

Mansbach, R. A., S. Chakraborty, T. K. Nguyen and S. Gnanakaran. Differential molecular signatures of the D and G forms the SARS-CoV2 trimeric Spike protein. Submitted to *Science Advances*. (LA-UR-20-25181)

Presentation Slides

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

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)

Posters

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)

Kubicek-Sutherland, J. Z., J. P. Theiler, K. Yusim, B. T. Foley, C. A. Lopez Bautista, S. Gnanakaran and H. Mukundan. Targeting Amphiphilic Biomarkers from Emerging Pathogens for Detection and Therapeutic Applications. Presented at *2019 Chemical and Biological Defense Science & Technology (CBD S&T) Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-31352)

Particle Modeling of High-Altitude Nuclear Explosions

Ari Le
20200334ER

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.

Publications

Journal Articles

Le, A. Y., D. Winske, A. J. Stanier, W. S. Daughton, M. Cowee, B. A. Wetherton and F. Guo. Astrophysical explosions revisited: collisionless coupling of debris to magnetized plasma. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-20-30244)

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)

Stanier, A., L. Chac\xc3\xb3n and A. Le. A cancellation problem in hybrid particle-in-cell schemes due to finite particle size. 2020. *Journal of Computational Physics*. **420**: 109705. (LA-UR-19-32264 DOI: 10.1016/j.jcp.2020.109705)

Tang, B., W. Li, D. B. Graham, C. Wang, Y. V. Khotyaintsev, A. Y. Le, B. Giles, P. A. Lindqvist, R. E. Ergun and J. L. Burch. Lower hybrid waves at the magnetosheath separatrix region. Submitted to *Geophysical Research Letters*. (LA-UR-20-27264)

Reports

Le, A. Y., D. Winske, W. S. Daughton and A. J. Stanier. Ion Kinetics in High-Altitude Nuclear Explosions. Unpublished report. (LA-CP-20-20023)

Presentation Slides

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

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., D. Winske, M. Cowee, A. J. Stanier and W. S. Daughton. HANE Modeling with Hybrid VPIC at LANL. Presented at *DTRA HiEx Technical Exchange Meeting*, Los Alamos, New Mexico, United States, 2020-01-29 - 2020-01-29. (LA-UR-20-20737)

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., 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)

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)

Capturing the First Uranium Alkylidene Complex

Jaqueline Kiplinger
20200338ER

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.

Next Steps to Molecular Actinide Nitrides

Marisa Monreal
20200435ER

Project Description

This project is comprised of fundamental chemistry research, specifically actinide synthetic chemistry, with a high-level goal of contributing to the understanding of the chemical behavior of nuclear fuels. This work thus addresses national security challenges in nuclear energy. The main expected outcomes will be major advancements to the field of fundamental actinide chemistry, but the project's results are also expected to benefit nuclear fuels research. Therefore, this research will impact Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions in scientific discovery and innovation, nuclear energy, and energy security.

Powering the Resolution Revolution with Multi-Resolution Algorithms: Merging Image Analysis, Molecular Simulation and Model Building

Karissa Sanbonmatsu
20180139ER

Project Description

Fundamental biology science and health security have important applications in national security. Molecules in living systems and biomedicine have highly intricate, complex structures and shapes. Their shape often determines how they work and the role they play in our own bodies and in harmful bacteria. If we can understand how these molecules work in atomic detail, we may be able to control them, laying the foundation for new drugs to treat disease and to defend against harmful bacteria. This field is called structural biology. To date, structural biology has played an instrumental role in almost every aspect of life science and biomedicine. This project focuses on cryogenic electron microscopy, a technique revolutionizing the field of structural biology. By satisfying the large demand for computational tools in cryogenic electron microscopy, our project stands to position Los Alamos National Laboratory at the forefront of a revolution in structural biology.

Technical Outcomes

This project automated the process of 3-dimensional modeling for structural biology data, enabling researchers to automatically produce all-atom models for many different datasets. This was accomplished by integrating molecular simulation with cryogenic electron microscopy (cryo-EM), using the experimentally measured electron density as a bias, resulting in all-atom models fully consistent with the experimental data. Because the force field is defined by the initial structural model, it preserves the stereochemistry, while producing excellent fits to the data.

Publications

Journal Articles

*Jung, J., W. Nishima, M. Daniels, G. Bascom, C. Kobayashi, A. Adedoyin, M. Wall, A. Lappala, D. Phillips, W. Fischer, C. Tung, T. Schlick, Y. Sugita and K. Y. Sanbonmatsu. Scaling molecular dynamics beyond 100,000 processor cores for large-scale biophysical simulations. 2019. *Journal of Computational Chemistry*. **40** (21): 1919-1930. (LA-UR-18-31413 DOI: 10.1002/jcc.25840)

Kim, D. N., B. Thiel, T. Mrozowich, S. P. Hennelly, I. Hofacker, T. Patel and K. Y. Sanbonmatsu. CNBP alters 3-D structure of lncRNA Braveheart in solution. Submitted to *Nature Communications*. (LA-UR-19-30307)

*Kim, D. N., N. W. Moriarty, S. Kirmizialtin, P. V. Afonine, B. Poon, O. V. Sobolev, P. D. Adams and K. Sanbonmatsu. Cryo_fit: Democratization of flexible fitting for cryo-EM. 2019. *Journal of Structural Biology*. **208** (1): 1-6. (LA-UR-19-31082 DOI: 10.1016/j.jsb.2019.05.012)

Kim, D. N. and K. Y. Sanbonmatsu. Tools for the cryo-EM gold rush: going from the cryo-EM map to the atomistic model. Submitted to *Bioscience Reports*. (LA-UR-19-31083)

Posters

Lappala, A. Self-organization and compaction in biological and soft matter systems. Presented at *CNLS external review*, Los Alamos, New Mexico, United States, 2018-05-03 - 2018-05-03. (LA-UR-18-23790)

Geophysical Signatures of Changing Water Resources

Carene Larmat
20180158ER

Project Description

Water is necessary for all facets of life, and energy production and water resources are inextricably intertwined. Increasing strains on water resources due to groundwater withdrawals and frequent drought conditions, particularly in the US West, has the potential to threaten US energy production. By combining a set of non-traditional geophysical measurements, we will be able to quantify the distribution of groundwater resources and changes in them over time in response to changing meteorological conditions in a way that has not been possible previously, thereby improving understanding of energy security threats. Our results will have direct impact to the DOE cross-cutting initiative Water-Energy Nexus, as well as the Department of Energy Office of Energy Policy and Systems Analysis (EPSA) and Biological and Environmental Research (BER) programs.

Technical Outcomes

This project adapted seismic methods to document changes of subsurface properties covering a few decades and found changes related to groundwater in the Los Angeles area. The team also performed a joint inversion which results in a better estimate of water mass loss when adding gravity to ground deformation. This demonstrates that seismological and geophysical methods are indeed effective at monitoring temporal changes in the shallow subsurface, expanding their applications to energy production and water resources monitoring.

Publications

Journal Articles

Delorey, A. A. and E. M. Syracuse. Measuring Changes in Groundwater using a Joint Inversion of Gravity and Ground Deformation. Submitted to *Geophysical Research Letters*. (LA-UR-20-23718)

Syracuse, E. M., J. A. Kintner, A. A. Delorey and H. Goldberg. Seismological Monitoring of Groundwater Resources in the Los Angeles Region. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-20-26268)

Reports

Larmat, C. 2021 IC reports. Unpublished report. (LA-UR-21-22173)

Presentation Slides

Delorey, A. A., H. Goldberg, S. Son, C. N. L. Gammans and E. M. Syracuse. Monitoring Changes in Groundwater Storage with Gravity, Ground Displacement, and Seismic Observations. Presented at *American Geophysical Union*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31458)

Goldberg, H. Determining the cause and nature of anomalous Rayleigh wave H/V ratio measurements in southern California. Presented at *IRIS Virtual Meeting*, Los Alamos, New Mexico, United States, 2018-07-13 - 2018-07-13. (LA-UR-18-26221)

Syracuse, E. M. Seismic signatures of changing water resources. . (LA-UR-18-22629)

Syracuse, E. M., A. A. Delorey, H. Goldberg, J. A. Kintner, C. Larmat, K. Gao and J. Muir. Probing temporal changes in the subsurface using ambient seismic noise (and, life at a national lab). . (LA-UR-20-22005)

Syracuse, E. M., A. A. Delorey, H. Goldberg and J. B. Muir. Probing groundwater using Rayleigh wave ellipticity measurements in southern California. Presented at *American Geophysical Union Fall Meeting*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31586)

Posters

Goldberg, H. Determining the cause and nature of anomalous Rayleigh wave H/V ratio measurements in southern California. Presented at *Los Alamos National Lab Student Symposium*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-26184)

Syracuse, E. M., A. A. Delorey, H. Goldberg and J. B. Muir. Using Ambient-Noise Based Ellipticity and Delay Times to Probe Groundwater Changes in Southern California. Presented at *Seismological Society of America annual meeting*, Seattle, Washington, United States, 2019-04-24 - 2019-04-24. (LA-UR-19-23585)

Syracuse, E. M., A. A. Delorey and J. Muir. Seismic Signatures of Changing Water Resources. Presented at *Seismological Society of America Annual Meeting*, Miami, Florida, United States, 2018-05-15 - 2018-05-17. (LA-UR-18-24137)

Other

Syracuse, E. M. Ambient-noise-based Rayleigh wave measurements for the Los Angeles Basin. Dataset. (LA-UR-19-28317)

Syracuse, E. M., J. A. Kintner, A. A. Delorey and H. Goldberg. Ambient-noise-based Rayleigh wave velocity measurements for the Los Angeles Basin. Dataset. (LA-UR-20-26561)

Removing and Swapping Photoreceptors in Algae to Improve Biomass Yield

Shawn Starkenburg
20180393ER

Project Description

This project directly supports the energy security mission of DOE and NNSA. The major hurdle impeding renewable fuel sourcing from algae is cost. Therefore, research efforts focused on increasing algal yields will directly reduce the price of algal derived gasoline and other transportation fuels. The goal of this project is to improve the yield and lower the cost of algal biofuel production 2 fold to improve the state of technology to meet the DOE targets for renewable energy use.

Technical Outcomes

Technical outcomes include pursuit of a provisional patent on the the development of a neochrome expressing algae, expansion of genetic engineering tools and protocols for genetically modifying algae species used for commercial applications, and improved growth rate and improved starch and lipid accumulation in production algae species with applications in biofuels.

Publications

Journal Articles

*Deodato, C. R., S. B. Barlow, B. T. Hovde and R. A. Cattolico. Naked Chrysochromulina (Haptophyta) isolates from lake and river ecosystems: An electron microscopic comparison including new observations on the type species of this taxon. 2019. *Algal Research*. **40**: 101492. (LA-UR-19-20025 DOI: 10.1016/j.algal.2019.101492)

Sanchez, M., C. Payen, F. Cheong, B. Hovde, S. Bissonnette, A. Arkin, J. Skerker, R. Brem, A. Caudy and M. Dunham. Transposon insertional mutagenesis in reveals - acting effects influencing species-dependent essential genes. 2019. *Genome Research*. **29** (3): 396-406. (LA-UR-19-20026 DOI: 10.1101/gr.232330.117)

Reports

Negi, S., S. R. Starkenburg and R. T. (. Sayre. Productivity and bioproduct formation in phototropic knock/out mutants in micro algae. Unpublished report. (LA-UR-20-25287)

Presentation Slides

Hovde, B. Bioenergy Research @ Los Alamos National Lab. . (LA-UR-20-22337)

Posters

Hovde, B. Genome sequencing and analysis of two geographically distinct freshwater isolates of the genus Chrysochromulina: insights into haptophyte evolution. Presented at *The 8th International Conference on Algal Biomass, Biofuels and Bioproducts*, Seattle, Washington, United States, 2018-06-11 - 2018-06-13. (LA-UR-18-24953)

Hovde, B., M. M. A. Baysinger, J. A. Ohan and P. Nath. Generating gel microdroplets using microfluidics. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27823)

Mettler, J. G., T. Britton, S. Negi and B. Hovde. CRISPR-Directed Editing of Photoreceptor Genes to Improve Biomass Accumulation in Microalgae. Presented at *LANL Student Symposium*, Los alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-27135)

Mettler, J. G., T. Britton, S. Negi and B. T. Hovde. CRISPR-Directed Editing of Photoreceptor Genes to Improve Biomass Accumulation in Microalgae. Presented at *Algae Biomass Organization Symposium*, Houston, Texas, United States, 2018-10-14 - 2018-10-17. (LA-UR-18-29318)

Next Generation Models for Radial Diffusion of Energetic Electrons in the Earth's Radiation Belts

Michael Henderson
20180449ER

Project Description

This project supports development of capabilities for Space Situational Awareness (SSA) both in a predictive realm and in post-facto analyses of spacecraft anomalies (forensics). Accurate specification/prediction of the relativistic electron populations in the radiation belt is critical for understanding and mitigating threats to space-based assets. The enhancement of Los Alamos National Laboratory datasets used in this project also maintains and supports broader national security needs including space-based treaty verification activities on-going at the Laboratory and the ability to plan for future missions. The new models for the radial diffusion transport parameters that will result from this work will constitute a transformational advancement over what is currently available and will place the Laboratory at the forefront of this research area.

Technical Outcomes

This project developed and validated the first four-dimensional variational (4D-Var) data assimilation technique for extracting radial diffusion parameters directly from the observed evolution of the electron phase space density. The phase space density with uncertainties has been computed for the entire Van Allen Probes mission (active during 2012-2019) and the first estimates of the radial diffusion transport parameters as a function of all three "adiabatic invariants" have been derived from this extensive data set.

Publications

Journal Articles

*Albert, J. M., R. S. Selesnick, S. K. Morley, M. G. Henderson and A. C. Kellerman. Calculation of Last Closed Drift Shells for the 2013 GEM Radiation Belt Challenge Events. 2018. *Journal of Geophysical Research: Space Physics*. **123** (11): 9597-9611. (LA-UR-19-30975 DOI: 10.1029/2018JA025991)

Jaynes, A. N., A. F. Ali, S. R. Elkington, D. M. Malaspina, D. N. Baker, X. Li, S. G. Kanekal, M. G. Henderson, C. A. Kletzing and J. R. Wygant. Fast Diffusion of Ultrarelativistic Electrons in the OuterRadiation Belt: 17 March 2015 Storm Event. Submitted to *Geophysical Research Letters*. (LA-UR-19-30974)

*Ripoll, J. -., T. Farges, D. M. Malaspina, E. H. Lay, G. S. Cunningham, G. B. Hospodarsky, C. A. Kletzing and J. R. Wygant. Analysis of Electric and Magnetic Lightning-Generated Wave Amplitudes Measured by the Van Allen Probes. 2020. *Geophysical Research Letters*. **47** (6): e2020GL087503. (LA-UR-19-31568 DOI: 10.1029/2020GL087503)

Presentation Slides

Cunningham, G. S. Trapped Electrons in the Near-Earth Space Environment: a Golden Age for Radiation-Belt Physics. . (LA-UR-18-30486)

Godinez Vazquez, H. C. and M. G. Henderson. Data Assimilation for the Radiation Belt Environment. Presented at *SIAM Annual Meeting*, Portland, Oregon, United States, 2018-07-09 - 2018-07-13. (LA-UR-18-26293)

Godinez Vazquez, H. C. and M. G. Henderson. Data Assimilation for the Radiation Belt Environment using the Four-Dimensional Variational Method. Presented at *AGU Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32342)

Posters

Godinez Vazquez, H. C. and M. G. Henderson. Estimating Diffusion Coefficients using Variational Methods. Presented at *Geospace Environment Modeling (GEM) 2018 Summer Workshop*, Santa Fe, New Mexico, United States, 2018-06-18 - 2018-06-22. (LA-UR-18-25420)

Godinez Vazquez, H. C. and M. G. Henderson. Variational Data Assimilation for 1-D Radiation Belt Model. Presented at *The Geospace Environment Modeling workshop 2019*, Santa Fe, New Mexico, United States, 2019-06-24 - 2019-06-28. (LA-UR-19-26120)

Optimization Aware Uncertainty Quantification in Non-Linear Networked Systems

Sidhant Misra
20180468ER

Project Description

In systems of national importance, such as critical infrastructures, where optimization is leveraged to achieve optimal technical performance or economic efficiency, uncertainty creates significant risks. If uncertainty is not accounted for properly during the design and optimization process, the system might be vulnerable even to relatively minor disturbances. Addressing this problem requires Uncertainty Quantification (UQ) to characterize the impact of uncertainty in a mathematical form, as well as integration of the uncertainty characterization in UQ-Aware Optimization. Using nonlinear networked systems as the primary example, we will (i) develop new methods for UQ using non-traditional approaches based on powerful new ideas in modern optimization theory and the theory of Graphical Models and (ii) develop techniques that incorporate both existing and our advanced UQ methods into a larger optimization framework. Our work will make significant contributions to the general fields of UQ and optimization. In addition, these concepts are directly applicable to security assessment and optimization under uncertainty in non-linear infrastructure networks—an integral part of the Laboratory's work on critical infrastructure and energy security. The project is also aligned with other mission relevant non-linear networks, including epidemic spreading, analysis of social or communication networks, and interdiction of networks transporting contraband.

Technical Outcomes

This project explored several approaches for Uncertainty Quantification (UQ) methods and their integration into optimization. The main outcome is two new methods (i) sparse polynomial chaos expansion and (ii) machine learning accelerated UQ and optimization. The two methods demonstrated significant efficiency gains on large power systems benchmark cases. These constitute the first methods that are both accurate and efficient enough to obtain control policies for safe operation in the face of uncertainty within practically relevant time limit requirements.

Publications

Journal Articles

Lasserre, J. B. and T. Weisser. DISTRIBUTIONALLY ROBUST POLYNOMIAL CHANCE-CONSTRAINTS UNDER MIXTURE AMBIGUITY SETS. Submitted to *Mathematical Programming*. (LA-UR-19-29307)

Luchnikov, I., D. M. R. Metivier, H. Ouerdane and M. Chertkov. Super-relaxation of loads ensembles energy consumption in discrete phase space. Submitted to *arxiv, Energy Conversion and Management*. (LA-UR-19-27341)

*Marx, S., T. Weisser, D. Henrion and J. B. Lasserre. A moment approach for entropy solutions to nonlinear hyperbolic PDEs. 2020. *Mathematical Control & Related Fields*. **10** (1): 113-140. (LA-UR-19-21398 DOI: 10.3934/mcrf.2019032)

R. Metivier, D. M., M. D. Vuffray and S. Misra. Efficient Polynomial Chaos Expansion for Uncertainty Quantification in Power Systems. Submitted to *Electric Power Systems Research*. (LA-UR-19-30262)

Roald, L. A., K. Sundar, A. V. Zlotnik, S. Misra and G. Andersson. An Uncertainty Management Framework for Integrated Gas-Electric Energy Systems. Submitted to *Proceedings of the IEEE*. (LA-UR-20-20818)

Conference Papers

Misra, S., D. Molzahn and K. Dvijotham. Optimal adaptive linearizations of the AC power flow equations. Presented at *Power Systems Control Conference*. (Dublin, Ireland, 2018-06-11 - 2018-06-11). (LA-UR-17-29721)

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)

Ng, Y., S. Misra, L. A. Roald and S. N. Backhaus. Statistical Learning for DC Optimal Power Flow. Presented at *Power Systems Computation Conference*. (Dublin, Ireland, 2018-06-11 - 2018-06-11). (LA-UR-17-29722)

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *COLT 2019 : Computational Learning Theory*. (Phoenix, Arizona, United States, 2019-06-25 - 2019-06-29). (LA-UR-19-20925)

Wiesser, T., S. Misra and L. A. Roald. Chance-Constrained Optimization for Non-Linear Network Flow Problems. Presented at *Semi-Algebraic techniques for the Optimal Power Flow Problem and Stability Assessment of Power Systems*. (Paris, France, 2018-01-16 - 2018-01-16). (LA-UR-17-31414)

Presentation Slides

Marx, S., T. Weisser, D. Henrion and J. B. Lasserre. A moment approach to approximating functional solutions. Presented at *IPAM: Workshop on Operator Theoretic Methods in Dynamic Data Analysis and Control*, Los Angeles, California, United States, 2019-02-11 - 2019-02-11. (LA-UR-19-21339)

Misra, S. Learning for optimization. Presented at *Grid science winter school*, Santa Fe, New Mexico, United States, 2019-01-06 - 2019-01-06. (LA-UR-19-21079)

Weisser, T. Relaxations and Uncertainty Quantification for the Power Grid. . (LA-UR-19-26045)

Weisser, T. Tighter bounds for AC-OPF through rank-one convexification. Presented at *SIAM AG 2019*, Bern, Switzerland, 2019-07-09 - 2019-07-09. (LA-UR-19-26092)

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)

Weisser, T. and B. Legat. MomentOpt.jl. Presented at *JuliaCon 2019*, Baltimore, Maryland, United States, 2019-07-23 - 2019-07-23. (LA-UR-19-27744)

Weisser, T. and B. Legat. MomentOpt.jl. Presented at *ICCOPT 2019*, Berlin, Germany, 2019-08-05 - 2019-08-05. (LA-UR-19-27727)

Weisser, T. and C. J. Coffrin. JuliaMoments/JuMPMoments. Presented at *JuMP-dev Workshop 2019*, Santiago, Chile, 2019-03-12 - 2019-03-12. (LA-UR-19-22390)

First Real-time Measurements of Quantum States of Ultracold Neutrons (UCN)

Zehui Wang
20200643ER

Project Description

This work builds a scientific and technological foundation for Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions. Free neutrons are unmistakable signatures of nuclear materials that are of critical importance to DOE/NNSA. Even though neutrons are quantum states similar to electrons and photons, most of the neutron experiments and technologies only treat them as if they are classical states of matter like a point-like bullet. Significant technologies hurdles have now been overcome by Los Alamos and collaborators through the establishment of the unique Ultracold Neutron (UCN) source at the Los Alamos Neutron Science Center (LANSCE) over the past decades, and more recently real-time positive-sensitive detections of UCN that allow us to probe the wave functions of UCN for the first time. Successful effort as described here will open up a new quantum world of neutrons. Impact on the fundamental science such as physics beyond the standard model, and technology such as UCN quantum sensors for materials, including nuclear materials, are anticipated.

Technical Outcomes

This project has resulted in two breakthroughs. On the theoretical front, we predicted strong scattering of ultracold neutrons in several neutronic metamaterial structures. On the experimental front, we have developed one of the world's most compact neutron cameras. The two results form the bases for a new class of quantum neutron experiments and motivate new search for 2D quantum confined states of UCN, which have not been achieved yet in the Laboratory.

Publications

Journal Articles

Wang, Z., M. Demarteau, C. Morris and Y. Shih. Strong scattering and parallel guiding of ultracold neutrons. Submitted to *Physical Review*. (LA-UR-20-27262)

Machine Learning/Artificial Intelligence (ML/AI) and Rich Sampling Campaign for Training a Practical In Silico Protein Folding Machine

Geoffrey Waldo
20200651ER

Project Description

The ability to generate biologically-derived protein-based countermeasures against chemical and biological threats hinges on our ability to design and express/ produce these proteins for therapy, prevention, or intervention. Existing approaches use in silico design which doesn't know anything about whether the proteins will actually fold when produced in work-horse organisms, Escherichia (E.) coli or other cells. Many designs fail to fold, even if they are predicted to be very stable. Much effort is wasted screening failed designs. This project plans to train a machine learning network ahead of time, with many mutations of the protein and their experimentally-determined folding fitness. Once trained, the network should be able to predict which sequences are foldable, greatly accelerating the in silico design cycle.

Technical Outcomes

This project focused on the all beta-sheet fluorescent proteins which have intrinsic activity upon folding. Libraries of a red fluorescent protein were screened by fluorescence-activated cell sorting (FACS) and binned according to folding status using cell fluorescence as proxy for folding. These form the basis sequencing and generating training needed to help predict when sequences are foldable.

Decoding the Function of Detonators

Bryan Henson
20200663ER

Project Description

This project addresses questions of importance to weapons surety. Understanding the mechanism of detonator function is critical to understanding how those detonators will age. Additionally, understanding the mechanism of function of existing detonators will feed into our ability to design new detonators in the future.

Technical Outcomes

This project involved the application of new laboratory scale radiographic techniques to understand the function of existing Exploding Foil Initiator (EFI) technology. The capability established in this project has revealed elements of detonator function for the first time, and will inform questions regarding detonator stewardship, design and fabrication. Results of this work are already impacting mission work from hydrocode design to detonator observation by proton radiography.

Increasing Transport: The Next-Generation Electrolytic Oxide Reduction Cell

Marisa Monreal
20200674ER

Project Description

The goal of this work is to improve a new technology to generate plutonium metal for weapons production. Use of this technology at Los Alamos would not only have a significant impact on overall production efficiency, but would also result in a substantial reduction in cost and waste. This work will therefore impact missions in Nuclear Security and National Defense, specifically Nuclear Weapons: Safety, Security, and Reliability of the Nuclear Stockpile, as well as Nuclear Nonproliferation and Counterproliferation. The new technology to generate plutonium metal that is the focus of this project is “electrolytic oxide reduction” (EOR). While EOR is in use in industry for certain metals, there are no published reports on the EOR of the plutonium surrogate used for this study, and the EOR of plutonium itself has yet to be fully demonstrated or understood. Thus, the study of EOR in this project and the advances in understanding resulting from this work will have high impact on fundamental chemistry and materials science, and the Scientific Discovery and Innovation mission.

Technical Outcomes

The critical outcome of this project is the discovery that adding stirring to electrolytic oxide reduction experiment results in a race between cerium oxide reduction and failure mechanisms such as membrane failure and cell component reduction from dissolved calcium metal. It is suspected that the current density was insufficient to exceed other reaction mechanisms. A higher current may reduce the cerium oxide before the membrane fails.

Detection and Attribution of No-Analog Fire

Richard Middleton
20200690ER

Project Description

Catastrophic wildfires in California and Australia have been the costliest global natural disasters in 2018–2020 and future climate change is likely to exacerbate these devastating events. We theorize the emerging existence of no-analog fires—unprecedentedly frequent, bigger, and faster spreading fires—coupled with catastrophic societal and economic impacts. Such catastrophic fires are an emerging national security threat. We will adapt and apply nascent machine learning (ML) techniques to observations of California wildfires, climate and atmospheric conditions, ecosystem and land-use and land-cover change, and infrastructure such as power lines to determine whether we have already entered a no-analog fire regime (detection) and what the cause of recent trends is (attribution).

Technical Outcomes

The project developed new databases and new machine learning (ML) approaches to: (1) detect emerging spatiotemporal fire trends in California (~20,000 fires), and (2) attribute these changes to shifts in the fire environment, including climate change, fuel management, and ignition frequency. ML analyses successfully identified changes in climate attributes such as precipitation, runoff, and evapotranspiration that are impacting the temporal and spatial dynamics of the wildfire occurrences in California.

Fundamentals of Chemical Exchange for Advanced Isotope Separations

George Goff
20200691ER

Project Description

Many of the nation's important missions require uranium enriched in Uranium-235. Traditional technology to acquire stocks of enriched uranium (EU) has primarily been through gaseous diffusion and ultracentrifugation, which is an energy intensive process that relies upon conversion of the uranium sources into toxic and corrosive uranium hexafluoride (UF6) gas. In contrast, Chemical Isotopic Exchange (CIE) processes represent a possible solution to the nation's enrichment needs and have been demonstrated in the commercial fuel fabrication industry and elsewhere for the isotopic separation of uranium as a liquid-liquid or solid-liquid process. However, there is limited open literature about CIE for uranium and the specific details of the underlying complex chemistry required is absent. Therefore a fundamental understanding of the complicated chemical processes involved in CIE for uranium is still needed. This project will perform experiments designed to develop the fundamental scientific understanding of chemical isotopic fractionation critical to enabling the design of advanced uranium separations processes.

Technical Outcomes

This project successfully demonstrated and measured isotopic fractionation of uranium in solvent extraction processes and made important observations in the underlying mechanisms that control these processes. The team also successfully applied first principles electronic structure calculations to Chemical Isotopic Exchange (CIE) processes for the first time, and identified a new uranium(VI/V) system for future studies.

Tracking the Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) Epidemic Using the Evolutionary Rate

Thomas Leitner
20200694ER

Project Description

This project aims to track the developing Coronavirus (COVID-19) epidemic through measuring the virus evolutionary rate. This may give us a way to estimate the impact of prevention campaigns and other changes in the epidemiology that we otherwise would have difficulty to estimate. This project will explore and exploit our previous knowledge of how viruses are affected by the environment and how that affects the replication rate and selection pressure. It is within-host processes that affect the population level evolutionary rate, so our quest is to understand how spread, prevention, and treatments affect the virus replication cycle, and how that in turn affects the evolutionary rate.

Technical Outcomes

Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) evolved slower than other ribonucleic acid (RNA) viruses, nessesitating development of new statistically robust methodology. Our reanalyses of early reports during the coronavirus (COVID-19) epidemic revealed misleading reports on spread patterns and speculations on the origin of SARS-CoV-2.

Publications

Journal Articles

Leitner, T. K. and S. Kumar. Where did SARS-CoV-2 come from?. Submitted to *Molecular Biology and Evolution*. (LA-UR-20-24880)

Mavian, C., S. K. Pond, S. Marini, B. R. Magalis, A. M. Vandamme, S. Dellicour, S. Scarpino, C. Houldcroft, J. Villabona-Arenas, T. K. Paisie, N. S. Trov\xc3\xa3o, C. Boucher, Y. Zhang, R. H. Scheuermann, O. Gascuel, T. Lam, M. A. Suchard, A. Abecasis, E. Wilkinson, T. de Oliveira, A. I. Bento, H. A. Schmidt, D. Martin, J. Hadfield, N. Faria, N. D. Grubaugh, R. A. Neher, G. Baele, P. Lemey, T. Stadler, J. Albert, K. A. Crandall, T. K. Leitner, A. Stamatakis, m. Prosperi and M. Salemi. Letter to the Editor: Sampling bias and incorrect rooting make phylogenetic network tracing of SARS-COV-2 infections unreliable. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-23207)

Reports

Leitner, T. K. Tracking the SARS-CoV-2 Epidemic Using the Evolutionary Rate. Unpublished report. (LA-UR-20-26976)

Combating Antibiotic Resistance with Phage Therapy

Alan Perelson
20200695ER

Project Description

The spread of multidrug drug resistant (MDR) bacteria poses a global threat to humanity and our armed forces. A United Nations report in 2019 estimated that drug-resistant diseases could result in 10 million deaths per year by 2050. Recently, there have been a few case reports in which all known antibiotics have failed to clear an infection and another approach involving bacteriophage or simply phage was used. Phage are viruses that infect bacteria and some called lytic phages can kill them. There are significant gaps in our knowledge of using phage as therapeutics that this project will address, including optimal phage dose levels, dosing frequency, dosing duration, and routes of administrations. The project involves analyzing and mathematically modeling quantitative data collected during a clinical trial to be performed at University of California San Diego Medical School aimed at filling the knowledge gaps needed to help make phage therapy a practical method of treating antibiotic resistant infections. There is also a growing interest in this type of therapy by the biotech industry, which will benefit from this work.

Technical Outcomes

Due to the coronavirus pandemic the phage therapy clinical trial that was to provide data for this project was postponed. The project was thus redirected to developing models for the within-host dynamics of Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) that focused on the effects of antiviral therapy with one or more drugs and the time that therapy was initiated. This project also modeled how the virus spread from the nose to the lungs and within the lungs of an infected person.

Publications

Journal Articles

Czuppon, P., F. D\xc3\xa9barre, A. Gon\xc3\xa7alves, O. Tenaillon, A. S. Perelson, J. Guedj and F. Blanquart. Predicted success of prophylactic antiviral therapy to block or delay SARS-CoV-2 infection depends on the drug's mechanism of action. Submitted to *PLOS Computational Biology*. (LA-UR-20-23569)

Gon\xc3\xa7alves, A., J. Bertrand, R. Ke, E. Comets, X. De Lamballerie, D. Malvy, A. Pizzorno, O. Terrier, M. R. Calatrava, F. Mentr\xc3\xa9, P. Smith, A. S. Perelson and J. Guedj. Timing of Antiviral Treatment Initiation is Critical to Reduce SARS-CoV-2 Viral Load. 2020. *CPT: Pharmacometrics & Systems Pharmacology*. **9** (9): 509-514. (LA-UR-20-22735 DOI: 10.1002/psp4.12543)

Iwanami, S., K. Ejima, K. S. Kim, K. Noshita, Y. Fujita, T. Miyazaki, S. Kohno, Y. Miyazaki, S. Morimoto, S. Nakaoka, Y. Koizumi, Y. Asai, K. Aihara, K. Watashi, R. N. Thompson, K. Shibuya, K. Fujiu, A. S. Perelson, S. Iwami and T. Wakita. Detection of significant antiviral drug effects on COVID-19 with reasonable sample sizes in randomized controlled trials: a modeling study combined with clinical data.. Submitted to *PLOS Medicine*. (LA-UR-20-23960)

Ke, R., C. Zitzmann, R. M. Ribeiro and A. S. Perelson. Kinetics of SARS-CoV-2 infection in the human upper and lower respiratory tracts and their relationship with infectiousness. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-27561)

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)

Posters

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

Investigation of Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) Interaction for Development of Lung-protective Therapies

Sofiya Micheva-Viteva
20200696ER

Project Description

Coronavirus (COVID-19) is the first pandemic in modern times that posed a risk to our National Security by inflicting Public Health Emergency and driving economic recession with a dangerous trajectory to global depression. Finding effective medication to curtail the disease will protect Public Health and strengthen the Economy and National Security. Our research provides a path to fundamental understanding of the COVID-19 pathology that brings people to intensive care units. The scientific discovery originating from this research will speed up the development of therapeutics that will relieve the deadly Severe Acute Respiratory Syndrome (SARS) pathology and curtail future coronavirus pandemics. This project seeks to investigate the ability of the current Coronavirus-2 to cause tissue damage even when it is not growing within the host cells. This breakthrough scientific discovery will help the ongoing clinical studies of therapeutics and vaccines for COVID-19 by providing fundamental knowledge of underlining mechanisms that will determine the success or failure of the treatment.

Technical Outcomes

This project established a cell-based system to investigate the interaction between coronavirus-2 (CoV2) particles with human angiotensin-converting enzyme2 (ACE2). The team found that binding of non-replicating viral particles or antibodies specific to the ACE2 receptor activated inflammatory responses and induced malignancies associated with the pathology of corona virus infection disease, including fibrosis and deoxyribonucleic acid (DNA) damage. Small molecule developed as a countermeasure to hypertension was capable to reduce inflammation in the in vitro cell model.

Publications

Journal Articles

Micheva-Viteva, S. N., A. S. Bell and S. R. Starkenburg. JNK-Thr187 signaling at the interface of autophagy and cell survival is essential for infectious Influenza A virus particle production by lung carcinoma and normal human bronchial epithelial cells in vitro. Submitted to *Viruses*. (LA-UR-20-30117)

Presentation Slides

Cirigliano, E. and S. N. Micheva-Viteva. The role of ACE2 in SARS-CoV-2 induced pathologies. Presented at *2020 LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25485)

Informing Mitigation Strategies for Coronavirus (COVID-19)

Carrie Manore
20200697ER

Project Description

The Coronavirus (COVID-19) pandemic is of immediate national security concern, and chief among the questions that need to be answered is how best to control the spread, ensure that our medical facilities are not overwhelmed, and minimize death and illness using non-pharmaceutical interventions such as social distancing, increased hygiene, and school closures. This project will develop epidemiological models that can be applied to directly answering these questions and adapted to particular locations across population, age structure, and available interventions. The models will be tested on past and ongoing outbreaks and then used to inform best strategies going forward both for controlling outbreaks or preventing them in locations without community spread. This is critical for the health of the United States and the world.

Technical Outcomes

This project informed mitigation strategies for Coronavirus (COVID-19) to provide decision makers with what-if scenarios in time to prevent infections and loss of life.

Publications

Journal Articles

Castro, L. A., C. D. Shelley, D. A. Osthus, I. J. Michaud, J. Mitchell, C. A. Manore and S. Y. Del Valle. How New Mexico Leveraged a COVID-19 Case Forecasting Model to Preemptively Address the Healthcare Needs of the State: A Quantitative Analysis. Submitted to *JMIR Public Health and Surveillance*. (LA-UR-21-21597)

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. Submitted to *Health Policy OPEN*. (LA-UR-20-30424)

Shea, K., C. A. Manore, S. Y. Del Valle, I. K. Crooker, G. Fairchild, T. C. Germann, R. C. Rael, C. M. Watson Ross and J. A. Spencer. COVID-19 reopening strategies at the county level in the face of uncertainty: Multiple Models for Outbreak Decision Support. Submitted to *Science*. (LA-UR-20-27777)

Shelley, C. D., P. S. Chadwick, C. A. Manore and S. Y. Del Valle. Safely Reopening K-12 Schools During the COVID-19 Pandemic. Submitted to *Epidemics*. (LA-UR-20-27585)

Presentation Slides

Manore, C. A. Covid-19 Modeling for Pandemic Response. Presented at *Joint Mathematical Meetings*, Remote, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20113)

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. Reopening K-12 Schools During the COVID-19 Pandemic. . (LA-UR-20-27067)

Spencer, J. A. Prioritizing Mitigation Strategies for COVID-19. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-26077)

Spencer, J. A., C. A. Manore and H. J. Wearing. Prioritizing Mitigation Strategies for COVID-19 in New Mexico. Presented at *Society for Mathematical Biology Annual Meeting 2020*, Santa Fe, New Mexico, United States, 2020-08-20 - 2020-08-20. (LA-UR-20-26421)

Spencer, J. A., H. Wearing and C. A. Manore. Comparative Dynamics of Five Common Human Viruses Contributing to Seasonal Influenza-like Illness. Presented at *Ecological Society of America Annual Meeting*, Salt Lake City, Utah, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-25525)

Spencer, J. A. and K. Martinez. Mitigation and Data Fusion Approaches to Understanding Infectious Diseases. Presented at *Challenges in Biomathematical Modeling*, Los Alamos, New Mexico, United States, 2020-09-17 - 2020-09-17. (LA-UR-20-27246)

Developing a National Spatial-Temporal Epidemiology Model for Decision Support

Paul Fenimore
20200699ER

Project Description

The project seeks to build a high resolution national spatial-temporal disease propagation model. This model exploits knowledge of within host disease progression, and how interventions impact that progression to provide a tool that can rapidly run many scenarios to quantify the value of interventions. This tool is essential for the bio-security mission at Los Alamos, as it will be used to inform government decision makers about course of action is best for the country.

Technical Outcomes

This project integrated added realism to epidemic spatio-temporal models by incorporating road networks and more realistic disease progression parameters. The result is a model that was used to provide situational awareness to the governor of New Mexico.

Publications

Journal Articles

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. Submitted to *The Lancet, Global Health*. (LA-UR-21-21361)

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. Submitted to *The Lancet, Global Health*. (LA-UR-21-21361)

Hengartner, N. W., I. Torres, E. Romero-Severson, R. Mahesh, N. R. Ortega, R. Ke and L. Cuellar-Hengartner. Assessing the Impact of Human Mobility to Predict Regional Excess Death in Ecuador. Submitted to *United Nation Development Program Report*. (LA-UR-21-21098)

Hengartner, N. W., I. Trejo Lorenzo and A. Patrick. Nonparametric estimation of the reproductive rate in generalized SEIR models. Submitted to *PLOS One*. (LA-UR-20-30505)

Trejo Lorenzo, I. and N. W. Hengartner. A modified Susceptible-Infected-Recovered model for observed under-reported incidence data. Submitted to *PLOS One*. (LA-UR-20-30041)

Presentation Slides

Hengartner, N. W. V&V for COVID-19 Decisions. Presented at *ASME Verification & Validation Symposium*, Virtual, New Mexico, United States, 2020-05-21 - 2020-05-22. (LA-UR-20-23823)

Forecasting Confirmed Cases and Deaths for Coronavirus (COVID-19)

David Osthus
20200700ER

Project Description

Public health security is national security and global security. Coronavirus (COVID-19) is producing a pandemic the likes of which we haven't seen since the 1918 Spanish flu which killed over half a million people in the United States (US) and over 50 million people worldwide. Accurate information is critical for decision makers to act upon. Currently, a real-time COVID-19 forecasting model does not exist. This project will build one and disseminate the forecasts to the public, filling an informational vacuum while providing decision makers with useful information for both planning and assessing the effectiveness of previous interventions. The forecasting model will produce forecasts for all US states, as well as all countries with at least one confirmed case.

Technical Outcomes

This project developed and deployed a coronavirus forecasting model on a public-facing website within two weeks of receiving funding, providing valuable information to public health officials and the public at-large at the time it was most needed. At its peak, the website was getting 20 thousand visits a week. The forecasts on the website are being used to support the United States Centers for Disease Control and Prevention (CDC) and the New Mexico Department of Health (DOH).

Publications

Journal Articles

Bracher, J., D. Wolffram, J. Deuschel, K. Gorgen, J. Ketterer, A. Ullrich, S. Abbott, M. Barbarossa, D. Bertsimas, S. Bhatia, M. Bodych, N. Bosse, J. P. Burgard, L. A. Castro, G. Fairchild, J. Fuhrmann, S. Funk, K. Gogolewski, Q. Gu, S. Heyder, T. Hotz, Y. Kheifetz, H. Kirsten, T. Krueger, E. Krymova, M. Li, J. Meinke, I. J. Michaud, K. Niedzielewski, T. Ozanski, F. Rakowski, M. Scholz, S. Soni, A. Srivastava, J. Zieli\xc5\x84ski, D. Zou, T. Gneiting and M. Schienle. Short-term forecasting of COVID-19 in Germany and Poland during the second wave - a preregistered study. Submitted to *Nature Communications*. (LA-UR-21-20048)

Castro, L. A., C. D. Shelley, D. A. Osthus, I. J. Michaud, J. Mitchell, C. A. Manore and S. Y. Del Valle. How New Mexico Leveraged a COVID-19 Case Forecasting Model to Preemptively Address the Healthcare Needs of the State: A Quantitative Analysis. Submitted to *JMIR Public Health and Surveillance*. (LA-UR-21-21597)

Cramer, E. Y., D. A. Osthus, L. A. Castro, G. Fairchild, I. J. Michaud and N. G. Reich. Evaluation of individual and ensemble probabilistic forecasts of COVID-19 mortality in the US. Submitted to *Epidemics*. (LA-UR-21-20490)

Ray, E. L., N. Wattanachit, J. Niemi, A. H. Kanji, K. House, E. Y. Cramer, J. Bracher, A. Zheng, T. K. Yamana, S. Woody, Y. Wang, R. L. Walraven, V. Tomar, K. Sherratt, D. Sheldon, B. A. Prakash, D. A. Osthus, M. L. Li, E. C. Lee, U. Koyluoglu, P. Keskinocak, Y. Gu, Q. Gu, S. Corsetti, J. Chhatwal, H. Biegel, M. Ben-Nun, J. Walker, R. Slayton, V. Lopez, M. Biggerstaff, M. A. Johansson and N. G. Reich. Ensemble Forecasts of COVID-19 in the U.S.. Submitted to *JAMA*. (LA-UR-20-26092)

Reports

Castro, L. A., G. Fairchild, I. J. Michaud and D. A. Osthus. COFFEE: COVID-19 Forecasts using Fast Evaluations and Estimation. Unpublished report. (LA-UR-20-28630)

Presentation Slides

Castro, L. A. The evolution of COVID-19 forecasting: What went right, what went wrong, and how do we do better next time. . (LA-UR-21-20686)

Fitch, J. P. Multidisciplinary R&D to Improve COVID-19 Understanding and Response. Presented at *Washington State Univ.*, Pullman, Washington, United States, 2020-10-15 - 2020-10-15. (LA-UR-20-26408)

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)

Osthus, D. A. Forecasting Methodologies for COVID-19 for the U.S. States and Globally. . (LA-UR-20-23311)

Osthus, D. A. LANL COVID-19 Forecasting Model. . (LA-UR-20-23519)

Osthus, D. A. and L. A. Castro. LANL’s COVID-19 Confirmed Cases, Deaths, and Hospitalizations Forecasting Model. . (LA-UR-20-23520)

Design and Syntheses of Surface Epitope Peptides and Peptide Mimetic Motives for Pan-Corona Vaccines

Jurgen Schmidt
20200705ER

Project Description

Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2), a ribonucleic acid (RNA) virus of the corona family, is the causative agent of COVID-19. Vaccines against the infection and antibodies for early detection are direly needed. Conserved regions on viral surfaces are ideal targets to induce immune response required for vaccines, as well as, antibody development for detection purposes. However, the use of full viral attenuated vaccine is time consuming and needs extensive validation before use. This project proposes that an antigen for vaccines based on only the peptide epitopes of the viral surface can be deployed more rapidly. This project aims to synthesize the peptides and protein fragments identified in a collaborative effort with University of Texas medical Branch (UTMB) for vaccines and detection antibodies using advanced de novo microwave syntheses. The methods deployed follow and expand upon protocols co-developed with our collaborators at UTMB for alpha and filo virus families shown to be effective in rapidly generating guide sequences. The team will then work with UTMB to demonstrate a cross-reactive pan-corona virus family vaccine response that can lead to broad-spectrum corona virus counter-measures against current and future iterations of corona viral challenges.

Technical Outcomes

The S1 region of the Corona spike contains the Recognition Binding Domain (RBD) making the first contact of the virus with a host Angiotensin Converting Enzyme (ACE) transmembrane receptor essential for viral docking to host cell surface. This project carefully selected immunogenic short epitopes that were used to design and deploy synthetic peptides representing Severe Acute Respiratory Syndrome (SARS) Spike protein. The results suggest these can be used as rapidly deployable emergency vaccines and for differential diagnosis.

Publications

Journal Articles

Schmidt, J. G., C. H. Schein, E. S. Anaya, W. Braun, S. S. Negi, S. Dreskin Cori Levine and S. McClellan. Synthetic antigens for detection of Covid-19 infections. Submitted to *bioXriv followed by publication in PLOS*. (LA-UR-21-20606)

Strategies for Coronavirus Vaccines to Protect Against the Current Pandemic Strains and Emergent Zoonoses

Bette Korber
20200706ER

Project Description

This project's team has expertise in vaccine design against diverse viruses and in modeling antibody/protein interactions. The team designed the human immunodeficiency virus (HIV) "mosaic" vaccine antigens that elicited a high degree of protection in rhesus macaques, that are now being tested in human clinical trials. The team also created a computational vaccine design strategy called Epigraphs. Epigraph filovirus vaccines fully protect against lethal Ebola and Marburg virus disease in mice and show promise against influenza. This project will design a novel coronavirus vaccine that may be helpful against the current pandemic virus, Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2, which causes COVID-19), to be tested in parallel with efforts already underway by the team's colleagues at Duke, Harvard, and University of Pennsylvania. The project will also create two distinctive design strategies that have the potential to provide protection against future coronavirus outbreaks. As COVID-19 is the third major human coronavirus outbreak of the 21st century, this is a vital goal to protect global health security. Finally, the project will create a bioinformatics pipeline to track mutations as they arise, with the intention of identifying mutations that could confer resistance to immune responses to vaccines that are under development.

Technical Outcomes

This project designed a conserved region vaccine for T cell responses using Epigraph that is immunogenic in mice and under further testing at Harvard. The team built the tools to develop the public cov.lanl.gov website, designed reagent panels for evaluating therapeutic antibodies and vaccine sera, and incorporated the emergent data into vaccine design ideas. The team also did preliminary analysis of betacoronavirus evolution to enable submission of a National Institutes of Health (NIH) Research Program Project (P01) proposal to design a pan-betacoronavirus vaccine.

Publications

Journal Articles

*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)

Mansbach, R. A., S. Chakraborty, T. K. Nguyen and S. Gnanakaran. Differential molecular signatures of the D and G forms the SARS-CoV2 trimeric Spike protein. Submitted to *Science Advances*. (LA-UR-20-25181)

Nguyen, T. K., S. Chakraborty, R. A. Mansbach, B. T. M. Korber and S. Gnanakaran. Exploring the role of glycans in the interaction of SARS-CoV-2 RBD and human receptor ACE2. Submitted to *MDPI Pathogens*. (LA-UR-21-22583)

Weissman, D., M. Alameh, C. C. Labranche, R. J. Edwards, L. Sutherland, S. Santra, K. Mansouri, S. Gobeil, C. McDanal, N. Pardi, M. J. Mulligan, K. E. Lyke, N. Kitchin, J. Absalon, A. Gurtman, S. Lockhart, K. Neuzil, V. Raabe, R. Bailey, K. A. Swanson, P. Li, K. Koury, W. Kalina, D. Cooper, C. Fontes-Garfias, P. Shi, \. Tu\xcc\x88reci, K. R. Tompkins, E. E. Walsh, R. Frenck, A. R. Falsey, P. R. Dormitzer, W. C. Gruber, P. A. Shaw, M. G. Lewis, U. Sahin, K. U. Jansen, P. Acharya, B. F. Haynes, B. T. M. Korber and D. C. Montefiori. D614G Spike Mutation Increases SARS CoV-2 Susceptibility to Neutralization. 2020. *Cell Host & Microbe*. (LA-UR-20-25579 DOI: 10.1016/j.chom.2020.11.012)

Presentation Slides

M. Korber, B. T. The D614G mutation in Spike: increased infectivity and neutralizing Ab sensitivity and the underlying mechanism. . (LA-UR-20-27323)

Phylodynamic Methods for Actionable Understanding of the Coronavirus (COVID-19) Pandemic

Emma Goldberg
20200711ER

Project Description

The ongoing Coronavirus (COVID-19) pandemic is a destabilizing influence across the globe. This project's research goals are to analyze viral genetic sequence data---which provide a relatively faithful report of viral spread---to provide key pieces of information that will guide an efficient public health response. This information includes estimating the true number of infected people---both confirmed and unknown cases---in a region, and identifying the extent to which increased case counts are due to community spread versus travel from other regions.

Technical Outcomes

This project developed an analysis procedure that uses genetic sequence data of the virus causing coronavirus to reveal properties of the epidemic within New Mexico. The team inferred unique introductions of the virus into the state over time, finding that they rose and then fell, even as new cases continued to rise. The team also identified sets of cases that resulted from each introduction and cross-checked those with state health department information to understand epidemiological links.

Publications

Presentation Slides

Goldberg, E. E. Phylogenetic Methods for COVID-19 Epidemiology. Presented at *Los Alamos - Arizona Days*, virtual, Arizona, United States, 2020-05-18 - 2020-05-18. (LA-UR-20-23672)

Goldberg, E. E. Inferring COVID-19 epidemiology from the phylogenetic tree of viral relationships. Presented at *Texas A&M Industrial and Applied Math (SIAM) Seminar*, (online), Texas, United States, 2020-10-12 - 2020-10-12. (LA-UR-20-27983)

Designing Reusable Smart Personal Protective Equipment (PPE) to Fight The Next Pandemic

Kumkum Ganguly
20200712ER

Project Description

As Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2, which causes COVID-19) explodes, the world races to mask up. The COVID-19 pandemic exposed unprecedented challenges regarding the shortage of personal protective equipment (PPE), especially N (non-oil) 95 masks, compromising the safety of health care workers and consequently our ability as a Nation to respond to this crisis. Several studies have reported different procedures for disinfecting the filtering face piece respirator before reuse, but with limited success. This project will evaluate the use of ionizing radiation e.g., X-ray, as a potential sterilizing technique for N95 masks and other PPE and its impact on material durability, particulate filtration efficiency, and pathogen inactivation. The data obtained will help in designing reusable PPE which can be sterilized by radiation and will be mission ready. The novelty of our multi-disciplinary approach is the thorough comparison of the sterilization procedures by ionizing radiation e.g., high energy X-ray and Gamma ray, as a control in the context of quantitation of pathogen inactivation and evaluation of the degradation of operational integrity of the N95 filters and other PPE materials and will be instrumental in designing radiation tolerant smart materials to produce PPE that can be easily sterilized and reused.

Technical Outcomes

The response to the Coronavirus pandemic has reached a critical juncture where frontline medical staffs are clamoring for face masks and personal protective equiptment (PPE). This multi-disciplinary approach compared sterilization procedures by ionizing radiation (e.g., high energy X-ray) and using Gamma ray as a control in the context of (i) quantitation of pathogen inactivation and (ii) evaluation of the degradation of operational integrity of the "N95" filters.

Rapid On-Demand Synthesis of Anti-Viral Favipiravir for the Treatment of Coronavirus (COVID-19)

Amanda Evans
20200717ER

Project Description

Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2, which causes COVID-19) is a new virus that is highly contagious with a high mortality rate. While anti-malaria drugs like hydroxychloroquine have been suggested to combat COVID-19, their effectiveness against this disease are unknown and their side effects are potentially very serious, inclusive of blindness and death. Therefore, it is imperative that we study and develop other anti-viral drugs that may help in the fight against COVID-19. Favipiravir is an anti-viral drug that has shown promise in early trials to combat COVID-19. The current synthetic routes to produce favipiravir are inefficient, provide low yields and require several days, making the process impractical for large-scale production. This project will develop a new, efficient process for the production of favipiravir that results in fewer steps, a reduction in manufacturing time, and higher yields by using a combination of batch and continuous flow chemistry processes. Success in this endeavor will allow for greater access to larger quantities of favipiravir for further studies and ultimately for patient treatment. If favipiravir proves as effective as initial trials indicate at fighting COVID-19, this drug could help save millions of lives, and significantly reduce suffering of those infected.

Technical Outcomes

This project investigated a five step flow/batch synthetic process for manufacturing favipiravir, an anti-viral that has been approved for treating coronavirus patients. Favipiravir has been approved for treating coronavirus in multiple countries - this project has focused on demonstrating a U.S.-based route that enables on demand manufacturing of favipiravir. This project's scalable and greener route to favipiravir allows us to isotopically label the molecule, in addition to securing a national path forward for making favipiravir.

Leveraging Los Alamos National Laboratory Personal Protective Equipment (PPE) Expertise to Inform Public Health Decisions Related to COVID-19

Michael Ham

20200720ER

Project Description

Combating the shortage of personal protective equipment (PPE) for Coronavirus (COVID-19) is a grave challenge facing America in these uncertain times. This project will devise ways to protect individuals and health care workers using novel PPE that targets the Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) and the way it spreads through our communities and hospitals. What people need is more information about which materials and methods are most effective and under what conditions they remain effective. Using our cutting edge diagnostics this project will fill in some of the missing information through detailed reports that help innovators make the smartest decisions for protecting the Nation from the virus. There are a lot of unknowns surrounding materials and methods and Americans need the guidance that the Laboratory can provide about the best materials and methods for creating the equipment that can protect them from the virus. The Lab's national security expertise is focused on keeping workers safe while building America's unmatched nuclear threat deterrent and will now be applied to fighting the latest threat to our way of life.

Technical Outcomes

The cutting edge diagnostics and novel methods this project invented tested the filtration efficiency and usability of novel materials for control of the droplets that spread Coronavirus (COVID-19). A cough machine that sprayed fluorescent dye was invented for the purpose of gaining an understanding of how materials might work when used as a mask. The results show surgical and cloth masks do a reasonable job of preventing large droplets, and the public would benefit from labeling mask performance.

Publications

Journal Articles

Ham, M. I., M. E. Moore, R. T. Williams, Y. Tao and E. A. Hillmer. How face masks can reduce community spread and create herd filtration efficiency. Submitted to *ACS Nano*. (LA-UR-20-30262)

Reports

Moore, M. E. and M. I. Ham. Estimating a protection factor from homemade facemasks for Los Alamos radioactive aerosols. Unpublished report. (LA-UR-20-26540)

Structural and Computational Identification of Potential Drugs Targeting Transmembrane Serine Protease 2 (TMPRSS2), a Host Protease Crucial for Coronavirus (COVID-19) Infection

Julian Chen
20200722ER

Project Description

This project addresses the immediate need for identifying potential drugs that can provide treatments for the Coronavirus (COVID-19) pandemic currently sweeping through the United States (US). By targeting a key host (human) protein mediating viral entry into the cell, and therefore infection, this project will use a mixed computational and experimental approach to rapidly identify already-approved Federal Drug Administration (FDA) drugs that could be deployed to treat infected individuals. This will add to the growing repertoire of identified compounds that could be part of a comprehensive prophylaxis / treatment plan for those infected with Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2), as well as vulnerable individuals, while vaccine development continues. This will also lay a foundation for efficiently and quickly addressing future pandemics, as well as protecting US interests around the world, including our military personnel.

Technical Outcomes

The human (host) protein transmembrane serine protease 2 (TMPRSS2) acts as a "gatekeeper", by priming the Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) and other viruses for entry into the cell. TMPRSS2 is therefore an attractive drug target for treating coronavirus. This project used computational methods to generate a theoretical model of TMPRSS2 and to screen chemical databases for potential molecules and drugs that bind to this model structure. TMPRSS2 has been expressed as an important step towards experimentally determining its three-dimensional structure.

Multiplex Assay Design for Respiratory Pathogens: Increasing Coronavirus (Covid-19) Testing Bandwidth

Jason Gans
20200732ER

Project Description

TaqMan polymerase chain reaction (PCR) testing is the gold-standard for detecting Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2), however existing lab infrastructure cannot keep up with the demand for testing. To address this challenge, this project will create a new multiplex SARS-CoV-2 TaqMan PCR assay that can test three times more patient samples than the current gold-standard Center for Disease Control and Prevention (CDC) assay, in the same amount of time. We will develop a second multiplex assay that can detect and differentiate SARS-CoV-2 from seven other common respiratory Ribonucleic Acid (RNA) viruses that can exhibit similar clinical manifestations. These new assays will be designed using sophisticated assay design software, previously developed at Los Alamos for biodefense pathogen detection. For existing assays, sensitivity predictions are essential for identifying new SARS-Cov-2 strains that might not be detected. We will develop a bioinformatics workflow that automates assay screening against current SARS-CoV-2 genomes and provides continuously updated, computational predictions of publicly available assay sensitivities. This will display the phylogenetic, temporal, and geographic information for any assay-genome combinations that are predicted to fail. Finally, the workflow will provide regularly updated PCR diagnostic assay designs that can replace failed SAR-CoV-2 detection assays.

Technical Outcomes

This project has produced experimentally validated Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) multiplex TaqMan Polymerase Chain Reaction (PCR) assay designs and developed two public web sites. The first site, already published in the journal Bioinformatics, provides near-real time, computational SARS-CoV-2 assay evaluations, while the second site automates and streamlines the submission of newly sequenced SARS-CoV-2 genomes to public databases. Finally, limits of TaqMan PCR multiplexing have been experimentally determined.

Publications

Journal Articles

Davenport, K. W., C. Lo, M. Shakya, M. C. Flynn, J. D. Gans, A. L. Myers y Gutierrez, B. Hu, P. Li, E. K. Player Jackson, Y. Xu and P. S. G. Chain. A Web Platform for Bioinformatics Analysis of SARS-CoV-2 Genomic Data. Submitted to *Bioinformatics*. (LA-UR-20-23331)

Davenport, K. W., P. Li, A. L. Myers y Gutierrez, M. C. Flynn, B. Hu, E. K. Player Jackson, M. Shakya, Y. Xu, J. D. Gans and P. S. G. Chain. A public website for the automated assessment and validation of SARS-CoV-2 diagnostic PCR assays. 2020. *Bioinformatics*. (LA-UR-20-23330 DOI: 10.1093/bioinformatics/btaa710)

Li, P., A. L. Myers y Gutierrez, K. W. Davenport, M. C. Flynn, B. Hu, C. Lo, E. K. Player Jackson, M. Shakya, Y. Xu, J. D. Gans and P. S. G. Chain. A Public Website for the Automated Assessment and Validation of SARS-CoV-2 Diagnostic PCR Assays. Submitted to *Bioinformatics*. (LA-UR-20-27750)

Shakya, M., P. S. G. Chain, K. W. Davenport, C. Lo, A. L. Myers y Gutierrez, P. Li, J. D. Gans, M. C. Flynn, E. K. Player Jackson, B. Hu and Y. Xu. EDGE COVID-19: A Web Platform to generate submission-ready genomes for SARS-CoV-2 sequencing efforts. Submitted to *Genome Research*. (LA-UR-20-24274)

Presentation Slides

G. Chain, P. S. Pandemic biosignatures: Using genomics to combat infectious diseases. Presented at *SOS Capability Review*, los alamos, New Mexico, United States, 2021-03-02 - 2021-03-04. (LA-UR-21-21646)

Quantifying the Within Host Dynamics of Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2)

Ruy Ribeiro
20200743ER

Project Description

Coronavirus (COVID-19) is an ongoing pandemic disease with vast impact in public health and the economy, with important potential implications for National security. Since it is a novel disease, there is much that is unknown in terms of its pathogenesis, progression, and management (for example, deployment of counter measures). This project will study the fundamental aspect of the dynamics of the virus within an infected person. It will model how the virus increases upon infection, is controlled and starts to decrease until it is eliminated from the organism. These models will give important insights into the evolution of disease, how severity depends on viral load, and the best use of novel antiviral drugs. This project can have an important impact on the Department of Energy's mission of “Science & innovation”, especially regarding to National security, by improving our knowledge and capabilities to control this viral infection. The results of this project can be integrated in population-level models to better predict the epidemiological spread of infection. The project will also keep Los Alamos National Laboratory at the forefront of research in this area.

Technical Outcomes

This project developed one of the first models of within-host dynamics of Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) in the upper (URT) and lower (LRT) respiratory tracts. This model was parameterized with clinical data, and provided important insights into the potential mechanism for virus maintenance in the LRT. The team also simulated the impact of different therapies on the course of the disease and proposed a new mechanistic model of virus transmission probability based on URT viral load.

Publications

Journal Articles

Gon\xc3\xa7alves, A., J. Bertrand, R. Ke, E. Comets, X. De Lamballerie, D. Malvy, A. Pizzorno, O. Terrier, M. R. Calatrava, F. Mentr\xc3\xa9, P. Smith, A. S. Perelson and J. Guedj. Timing of Antiviral Treatment Initiation is Critical to Reduce SARS-CoV-2 Viral Load. 2020. *CPT: Pharmacometrics & Systems Pharmacology*. **9** (9): 509-514. (LA-UR-20-22735 DOI: 10.1002/psp4.12543)

Ke, R., C. Zitzmann, R. M. Ribeiro and A. S. Perelson. Kinetics of SARS-CoV-2 infection in the human upper and lower respiratory tracts and their relationship with infectiousness. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-27561)

Posters

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

A Rapid Intermediate-Fidelity Indoor Flow and Transport and Dispersion Model for Predicting the Transmission of Infectious Diseases

Matthew Nelson
20200761ER

Project Description

The coronavirus (COVID-19) pandemic has interrupted critical operations both within the government and the private sector. We must learn how to resume these critical operations while minimizing the likelihood of transmission of COVID-19 between the staff that carry out these operations. Most of the guidance governing the resumption of normal operations has relied on simple social-distancing guidance, for example, maintaining 6 feet between individuals. This project will develop a new model by combining two existing models, which will allow us to explore the effect of heating, ventilation, and air conditioning (HVAC) vents on the effectiveness of the social distancing guidelines.

Technical Outcomes

This project translated the physics algorithms from QUICPLUME that affect the transmission of infectious diseases and have incorporated them into the Emergency Dose indoor model. The Emergency Dose code had not been touched for 12 years. The team was able to get it to compile but found the documentation on input files to be unclear and incomplete. We are working on filling in the knowledge gaps in the input files so it can execute a simulation successfully.

A Catalytic Acetylcholine Re–Activator as an Effective Countermeasure of Chemical Warfare Agent (CWA), Non-Traditional Agent (NTA), and Organophosphonate Exposures

Robert Williams
20200763ER

Project Description

Pesticides, Chemical Warfare Agents (CWAs), and recently declassified Fourth Generation Agents (FGAs or Novichoks) are among the most toxic small molecules known to man. These "nerve agents" prevent the normal function of human acetylcholinesterase (hAChE) by inactivating the enzyme's active site and preventing hydrolysis of acetylcholine (ACh) causing a rapid loss of neurotransmission, muscle paralysis, and death by suffocation. Oximes, such as 2-praldoxime chloride (2-PAM) are used to treat, stoichiometrically (1 oxime to 1 inhibited acetylcholinesterase), nerve agent intoxication; however, there are no current medical countermeasures (MCM) that can catalytically reactivate hAChE. This is important since a catalytic reactivator for hAChE would allow much lower doses of the MCM to be used, which are less toxic than currently employed in oxime therapy, as well as react much more rapidly than an oxime. To address this critical issue this project will develop a new, better, and innovative electrophilic, organometallic catalyst to restore the activity of hAChE and prevent the highly toxic effects caused by a nerve agent. This approach represents a paradigm shift since for the past seventy-five years only compounds similar to 2-PAM have been used as therapeutic countermeasures.

Technical Outcomes

Our overall objective is to produce a medical countermeasure against the effects of organophosphorous (OP) Chemical Warfare Agent (CWA) intoxication. As proof-of-concept, several ligands were synthesized and characterized as unique electrophilic catalysts. One PNP ligand-manganese catalyst exhibited the desired reaction with an OP-CWA surrogate compound. Further development of this catalyst type, operating with high catalytic turnover, is transformational. Several synthesized ligands with various metals are excellent candidates for further enhancement. These results extend efforts to counter emerging chemical threats.

Illuminating the Subsurface with Nonlinear Behavior

Andrew Delorey
20190552ECR

Project Description

The country's energy and environmental security depends on effective use of the subsurface because most of our energy comes from the subsurface and most of our waste material such as nuclear, brine (produced during oil and gas extraction) and CO2, is or will be stored in the subsurface. Despite this importance, we have very little timely information on subsurface conditions that affect the performance of these systems while avoiding hazards such as induced earthquakes and leakage of waste materials. Fractures at all scales are important to the performance of subsurface systems because they form the pathways for fluid migration and because their coalescence leads to earthquakes and containment failures. We are developing a new way to measure and monitor fractures in the subsurface using background seismic noise. As seismic waves travel through fractured materials, their travel times are perturbed by how weak or strong the contacts are across the fractures. Weak fracture contacts typically indicate that permeability is increasing and decreasing material strength, while stronger contacts typically indicate decreasing permeability and increasing material strength. These relationships have been observed in laboratory samples of rocks. Observing these relationships in the Earth will substantially contribute to our effective use of the subsurface.

Publications

Journal Articles

Delorey, A. A. Measuring Elasticity and Nonlinearity in the Earth using a Pump-Probe Analysis. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-20-28743)

Delorey, A. A. Measuring the Orientation of SHmax Using Nonlinary Elastic Behavior. Submitted to *Geophysical Research Letters*. (LA-UR-20-29378)

Presentation Slides

Delorey, A. A. Nonlinear Elastic Behavior from Laboratory to Earth Scale. . (LA-UR-19-31933)

Molecular Multi-Actinide Cores to Model Surface Reactivity

Aaron Tondreau
20190570ECR

Project Description

This project supports the safety, security, and reliability of the nuclear stockpile. This work will potentially inform decisions for long-term storage of actinides by inferring known reactivity of metal-surface surrogates via the cluster-surface analogy. This research will allow direct comparisons of the reactivity of small clusters of metal nuclei with known actinide surface reactivity. This will have implications for storage solutions attempting to mitigate known surface corrosion and chemical incompatibility concerns.

Publications

Journal Articles

Klamm, B. E., T. E. Albrecht-Schmitt, R. E. Baumbach, B. S. Billow, F. D. White, S. A. Kozimor, B. L. Scott and A. M. Tondreau. Using Intrinsic Lewis-Acidity in the Generation of Bimetallic Lanthanide Complexes. Submitted to *Inorganic Chemistry*. (LA-UR-20-21131)

Accurate Model for Predicting Mosquito Population Response to Weather and Water Management

Carrie Manore
20190581ECR

Project Description

Food security, health, and political stability are linked to coupled natural, climate, and human-engineered systems. This project will focus on mosquito-borne diseases that cause millions of deaths and hundreds of millions of illnesses globally every year. Accurately modeling mosquito populations and how they respond to weather, water management, and interventions is critical to quantifying risk, controlling outbreaks, and prevention of future outbreaks. Also, the United States has seen a 300% increase in cases of diseases spread by mosquitoes and ticks in the past decade. Since local and national government organizations are driven by minimizing risk and optimizing control, providing accurate mosquito forecasts will provide critical planning information. This project will develop an accurate model for predicting mosquito populations within-season using weather, water management, and demographic information. Models that couple water management and climate with mosquito habitat and populations will be critical to developing models coupling climate, weather, and mosquito dynamics to forecast mosquito-borne diseases, which are important to warfighter health, and to U.S. and global public health, with the potential to revolutionize prediction and planning for vector-borne disease risk now and in the future.

Publications

Journal Articles

Castro, L. A., E. N. A. Generous, W. Luo, A. Pastore y Piontti, K. M. Martinez, M. F. Gomes, D. A. Osthus, A. Ziemann, G. Fairchild, A. Vespignani, M. Santillana, C. A. Manore and S. Y. Del Valle. Using heterogeneous data to identify signatures of dengue outbreaks at fine spatial-temporal scales across Brazil. Submitted to *PLOS Neglected Tropical Diseases*. (LA-UR-20-29637)

Manore, C. A., K. C. Kempfert, K. Martinez, A. S. Siraj, J. R. Conrad, L. A. Castro, D. A. Osthus, E. N. A. Generous, N. K. Parikh, G. Fairchild, A. Ziemann and S. Y. Del Valle. Heterogeneous Data Fusion of Time Series to Nowcast Dengue at the State Level in Brazil. Submitted to *ArXiV*. (LA-UR-20-21471)

Manore, C. A., S. Y. Del Valle, E. N. A. Generous, K. Martinez, N. K. Parikh, D. A. Osthus and D. A. Romero-Alvarez. Google Health Trends performance to reflect dengue incidence in Brazilian states. Submitted to *BMC Infectious Diseases*. (LA-UR-19-31066)

Shutt, D. A., D. Goodsman, Z. J. L. Hemez, J. R. Conrad, C. Xu, D. A. Osthus, C. Russell, J. M. Hyman and C. A. Manore. A Process-Based Model with Temperature and Water Data Improve Predictions of Daily Mosquito Density. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-20732)

Presentation Slides

Fenimore, P. W., J. R. Mourant, J. R. Conrad, J. C. Miner, C. A. Manore, N. W. Hengartner, A. L. Atchley and B. H. Mcmahon. Project Review of EpiGrid: Comprehensive and Operational Model. . (LA-UR-19-20358)

Manore, C. A. Modeling Mosquitoes. Presented at *CMPD5*, Ft Lauderdale, Florida, United States, 2019-05-20 - 2019-05-22. (LA-UR-19-24635)

Manore, C. A., S. Y. Del Valle and D. A. Romero-Alvarez. Google Health Trends accuracy to reflect dengue incidence at the Brazilian states. Presented at *Meeting and conference*, Quito, Ecuador, 2019-07-22 - 2019-07-24. (LA-UR-19-26940)

Manore, C. A. and S. E. Michalak. Mathematics and Los Alamos National Laboratory: Advances and Collaboration. Presented at *ICIAM/SIAM*, Valencia, Spain, 2019-07-14 - 2019-07-19. (LA-UR-19-26713)

Shutt, D. A., S. Pankavich and A. Porter. Embedded ODE Model for the 2014 Ebola Outbreak in West Africa; An analysis of Guinea, Liberia & Sierra Leone. Presented at *2019 Annual Meeting Society for Mathematical Biology*, Montreal, Canada, 2019-07-22 - 2019-07-22. (LA-UR-19-22954)

Posters

Coronado, I. D. Mosquito-Borne Disease: A Worldwide Epidemic. . (LA-UR-19-28086)

Shutt, D. A., C. A. Manore, D. W. Goodsman, Z. J. L. Hemez, J. R. Conrad, C. Xu, J. M. Hyman and C. Russel. Heterogeneous Data Streams for Predicting Mosquito Density. Presented at *GS Symposium*, Los Alamos, New Mexico, United States, 2019-11-13 - 2019-11-13. (LA-UR-19-31203)

Spencer, J. A. and H. J. Wearing. Fitness Differences between Drug Resistant and Sensitive Strains of Mycobacterium tuberculosis. Presented at *Society for Mathematical Biology Annual Meeting*, Montreal, Canada, 2019-07-21 - 2019-07-26. (LA-UR-19-27013)

Drug Discovery by Automated Adaptation of Chemical Structure and Identity

Christopher Neale
20200543ECR

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.

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

Elena Giorgi
20200554ECR

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.

Publications

Journal Articles

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)

*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)

Posters

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

Photochemistry of Actinides in Ionic Liquids for Advanced Separations

Janelle Droessler

20200561ECR

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).

Computational and Experimental Bioprospecting of Algae for Antimicrobial Compounds

Blake Hovde

20200562ECR

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.

Advanced Understanding of Ocean Heat Storage by Coupling Large Eddy Simulation to a Global Ocean Model

Luke Van Roekel
20180549ECR

Project Description

Modeling the Earth System is a challenging, yet exciting, endeavor. There are physical processes essential to Earth System Models (ESMs) that span a wide range of sizes (meter to hundreds of kilometers). Present ESMs are unable to simulate this broad range of processes as many of these processes are smaller than the model grid cells. Newer ESMs that claim to be able to simulate a wider range of physical processes are unable to do so with high fidelity. This work will yield an unprecedented improvement in ESM ability to accurately simulate the rich tapestry of processes important to the ocean. This research will serve the energy security mission of DOE by helping to revolutionize our understanding and predictive capability of the migration and fate of carbon in the climate system. The resulting improved ESM fidelity will yield more confidence in any planning and policy that results from model predictions.

Technical Outcomes

The project developed a super-parameterized ocean model (runs a large eddy simulation (LES) to represent small scale turbulence regionally to understand coupling between the smallest scales of turbulence and the large scale ocean) and an Assumed Distribution Closure (combines the higher fidelity of LES with the lower computational cost of current models of oceanic turbulence). Both tools make model for prediction across scales (MPAS) and climate initiatives at Los Alamos more ready for Exascale computing

Publications

Journal Articles

Garanaik, A., R. Robey, L. Van Roekel and Q. Li. A Mass Flux Vertical Mixing Parameterization for the Ocean Surface Boundary Layer. Submitted to *Journal of Advances in Modeling Earth Systems*. (LA-UR-19-31170)

Li, Q. and L. Van Roekel. Towards Multiscale Modeling of Ocean Surface Turbulent Mixing Using Coupled MPAS-Ocean and PALM. Submitted to *Geoscientific Model Development*. (LA-UR-20-20427)

Posters

Li, Q. and L. Van Roekel. Towards Multiscale Modeling of Ocean Surface Turbulent Mixing Using Coupled MPAS-Ocean and PALM. Presented at *Ocean Sciences Meeting*, San Diego, California, United States, 2020-02-16 - 2020-02-21. (LA-UR-20-21454)

Modeling Heterogeneous Surveillance Data for Adaptive Real-time Response to Epidemics

Ethan Romero-Severson
20180612ECR

Project Description

Infectious disease outbreaks threaten local, national, and global security not only in their direct destabilizing effects, but also in their secondary effects by perceptions to governmental responses to those outbreaks. We propose that much of the data that is collected as part of routine surveillance can be used to move from a 'surveillance and reporting' paradigm to an active decision support framework where local outbreaks can be directly modeled and the potential efficacy and costs of alternative intervention programs can be tests in an evolving epidemic.

Technical Outcomes

This project made several technical advancements in moving towards surveillance as an active decision support framework. The team developed a method for dynamically partitioning surveillance data into local outbreaks based on comparison to a reference data set. The project also made several technical advancements in finding Dynamic Optimal Control Policies (DOCP) for epidemiological models that allow for dynamically updated optimal policies with real-world constraints. Finally, the team determined how to integrate clinical data into surveillance data analysis pipelines.

Publications

Journal Articles

*Bulla, I., I. H. Spickanll, D. Gromov and E. O. Romero-Severson. Sensitivity of joint contagiousness and susceptibility-based dynamic optimal control strategies for HIV prevention. 2018. *PLOS ONE*. **13** (10). (LA-UR-18-30123 DOI: 10.1371/journal.pone.0204741)

*Ezeonwumelu, I., I. Bartolo, F. Martin, A. Abecasis, T. Campos, E. O. Romero-Severson, T. Leitner and N. Taveira. Accidental Father-to-Son HIV-1 Transmission During the Seroconversion Period. 2018. *AIDS Research and Human Retroviruses*. **34** (10): 857-862. (LA-UR-19-25850 DOI: 10.1089/aid.2018.0060)

*Giardina, F., E. O. Romero-Severson, M. Axelsson, V. Svedhem, T. Leitner, T. Britton and J. Albert. Getting more from heterogeneous HIV-1 surveillance data in a high immigration country: estimation of incidence and undiagnosed population size using multiple biomarkers. 2019. *International Journal of Epidemiology*. **48** (6): 1795-1803. (LA-UR-19-25855 DOI: 10.1093/ije/dyz100)

*Goyal, A. and E. O. Romero-Severson. Screening for hepatitis D and PEG-Interferon over Tenofovir enhance general hepatitis control efforts in Brazil. 2018. *PLOS ONE*. **13** (9). (LA-UR-18-28686 DOI: 10.1371/journal.pone.0203831)

Gromov, D., I. Bulla, S. Serea and E. Romero-Severson. Numerical optimal control for HIV prevention with dynamic budget allocation.. Submitted to *Mathematical Medicine and Biology: A Journal of the IMA*. (LA-UR-19-30214)

*Gromov, D., I. Bulla and E. O. Romero-Severson. Systematic evaluation of the population-level effects of alternative treatment strategies on the basic reproduction number. 2019. *Journal of Theoretical Biology*. **462**: 381-390. (LA-UR-18-31251 DOI: 10.1016/j.jtbi.2018.11.029)

Leitner, T. K. and E. Romero-Severson. Phylogenetic patterns recover known HIV epidemiological relationships and reveal common transmission of multiple variants.. Submitted to *Nature Microbiology*. (LA-UR-19-30216)

*Leitner, T. and E. Romero-Severson. Phylogenetic patterns recover known HIV epidemiological relationships and reveal common transmission of multiple variants. 2018. *Nature Microbiology*. **3** (9): 983-988. (LA-UR-18-28043 DOI: 10.1038/s41564-018-0204-9)

*Romero-Severson, E., F. Giardina, T. K. Leitner, M. Axelsson, V. Svedhem and J. Albert. Getting more from heterogeneous HIV-1 surveillance data in a high immigration country: estimation of incidence and undiagnosed population size using multiple biomarkers. 2019. *International Journal of Epidemiology*. **48** (6): 1795-1803. (LA-UR-19-30213 DOI: 10.1093/ije/dyz100)

Romero-Severson, E., R. M. Ribeiro and M. Castro. Noise Is Not Error: Detecting Parametric Heterogeneity Between Epidemiologic Time Series. Submitted to *Frontiers in Microbiology*. (LA-UR-19-30215)

*Song, H., E. E. Giorgi, V. V. Ganusov, F. Cai, G. Athreya, H. Yoon, O. Carja, B. Hora, P. Hraber, E. Romero-Severson, C. Jiang, X. Li, S. Wang, H. Li, J. F. Salazar-Gonzalez, M. G. Salazar, N. Goonetilleke, B. F. Keele, D. C. Montefiori, M. S. Cohen, G. M. Shaw, B. H. Hahn, A. J. McMichael, B. F. Haynes, B. Korber, T. Bhattacharya and F. Gao. Tracking HIV-1 recombination to resolve its contribution to HIV-1 evolution in natural infection. 2018. *Nature Communications*. **9** (1): 1928. (LA-UR-19-30217 DOI: 10.1038/s41467-018-04217-5)

Presentation Slides

Romero-Severson, E. Next generation infectious disease surveillance. . (LA-UR-21-22649)

Joint Critical Thresholds and Extremes for Vulnerability Assessment of Regional Stability

Katrina Bennett
20180621ECR

Project Description

This project will address "what, where, how" of joint thresholds and extreme events (e.g. flooding+high temperatures) to provide a critical, climate-appropriate assessment of vulnerability to regional stability and security in US watersheds. The novel, science-based approach to vulnerability assessment in a no-analog future can be used to support decision-making for national security applications. The project also directly supports wider Department of Energy (DOE) challenges, including DOE Office of Science's focus on energy-water nexus and DOE's mission to provide actionable science to other federal agencies including the Department of Homeland Security and the Department of Defense.

Technical Outcomes

Changes in climate extremes and climate disturbances can cause catastrophic damage to social and ecological systems and are becoming increasingly common and intense at global and regional scales. This work to estimate changing extremes, using multiple statistical techniques, shows that extremes are projected to increase dramatically for the Colorado River basin, a critical watershed to the US economy. Adaptation measures can help planners and managers better prepare for changing extremes, reducing costs associated with damages.

Publications

Journal Articles

Bennett, K. E., B. Udall, S. Fleming and R. S. Middleton. The New Colorado River Basin. Submitted to *Nature Climate Change*. (LA-UR-20-28372)

Bennett, K. E., C. J. Talsma and R. Boero. Changes in Joint Extreme Hydroclimate Impacts in the Colorado River Basin. Submitted to *Water*. (LA-UR-20-27647)

*Bennett, K. E., G. Miller, C. Talsma, A. Jonko, A. Bruggeman, A. Atchley, A. Lavadie-Bulnes, E. Kwicklis and R. Middleton. Future water resource shifts in the high desert Southwest of Northern New Mexico, USA. 2020. *Journal of Hydrology: Regional Studies*. **28**: 100678. (LA-UR-19-30395 DOI: 10.1016/j.ejrh.2020.100678)

Bennett, K. E., J. Cherry, B. Balk and S. Lindsey. Using MODIS estimates of fractional snow cover area to improve streamflow forecasts in interior Alaska. 2019. *Hydrology and Earth System Sciences*. **23** (5): 2439-2459. (LA-UR-18-21603 DOI: 10.5194/hess-23-2439-2019)

Bennett, K. E., R. Boero and C. J. Talsma. Expectation of future natural hazards to joint extreme events in the Colorado River Basin.. Submitted to *Nature Climate Change*. (LA-UR-20-28365)

*Bennett, K. E., V. C. Tidwell, D. Llewellyn, S. Behery, L. Barrett, M. Stansbury and R. S. Middleton. Threats to a Colorado river provisioning basin under coupled future climate and societal scenarios. 2019. *Environmental Research Communications*. **1** (9): 95001. (LA-UR-18-30685 DOI: 10.1088/2515-7620/ab4028)

Meng, M., J. Macknick, V. Tidwell, K. E. Bennett and K. Sanders. Integrating water, energy, and climate modeling to assess vulnerabilities to the Western power grid. Submitted to *Environmental Research Letters*. (LA-UR-20-28368)

Talsma, C. J., K. E. Bennett, F. Yu and V. V. Vesselinov. Characterizing Extreme Events using Unsupervised Machine Learning Methods for Improved Understanding of Future Droughts in the Colorado River Basin. Submitted to *JGR Solid Earth, G-Cubed, Tectonics and Earth and Space Science*. (LA-UR-20-28366)

Tidwell, V., T. Lowry, T. Vandegrift, S. Behery, D. Llewellyn and K. E. Bennett. Importance of Water Infrastructure and Management Operations in Evaluating Impacts of Changing Climate and Water Use Regimes. Submitted to *Water Resources Research*. (LA-UR-20-28367)

Books/Chapters

Shrestha, R., K. E. Bennett, D. Peter and D. Yang. Hydrologic Extremes in Arctic Rivers and Regions: Historical Variability and Future Perspectives.. (LA-UR-20-28009)

Reports

Bennett, K. E. Drivers and feedbacks of joint cumulative extreme events: Advancing our understanding of hydro-ecologic perturbations in western US watersheds. Unpublished report. (LA-UR-19-23933)

Wagner, A. M., C. A. Hiemstra, G. E. Liston, K. E. Bennett, D. Cooley and A. B. Gelvin. Timing of Snowmelt and Intensity-Duration-Frequency Curves. Unpublished report. (LA-UR-21-21538)

Presentation Slides

Bennett, K. E., C. J. Talsma, R. Boero, J. R. Urrego Blanco and V. V. Vesselinov. Joint critical thresholds and extremes for vulnerability assessment of regional stability. Presented at *LANL COSIM Weekly Meeting*, Online, New Mexico, United States, 2020-07-01 - 2020-07-01. (LA-UR-20-28364)

Bennett, K. E., J. R. Urrego Blanco, C. J. Talsma and R. Boero. Joint critical hydroclimate extremes for vulnerability assessment of regional stability. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2018-12-10 - 2018-12-14. (LA-UR-20-28363)

Wagner, A., C. Hiemstra, G. E. Liston, D. Cooley and K. E. Bennett. Changes in Climate and its Effect on Timing of Snowmelt and Intensity-Duration-Frequency Curves. Presented at *SERDP In-Progress Review Meeting*, Online, District Of Columbia, United States, 2020-10-07 - 2020-10-07. (LA-UR-20-28369)

Molecular Basis of Ras-related Cancers

Angel Garcia
20170692PRD4

Project Description

We will use high performance computer simulations to model the interactions of cancer related proteins in environments that mimic the cell environment. We will study the interactions of oncogenes proteins with lipid membrane and with other proteins that, upon binding, activate the oncogenes. The nature of the interactions with the lipid bilayer and the activating proteins may offer opportunities to identify new targets for anti-cancer drug development. The computer simulations will be state-of-the-art atomistic molecular dynamics simulations. Larger scale models will also be used to study long time scale effects that are in time scales not accesible to atomistic simulations. Project collaborations include the National Cancer Institute and other National Laboratories.

Publications

Journal Articles

Ngo, A. V., H. Li, A. Mackerell, T. Allen, B. Roux and S. Noskov. Polarization Effects in Water-Mediated Selective Cation Transport Across a Narrow Transmembrane Channel. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-28023)

Unusual Oxidation States and Covalency-Tuning in Transuranic Molecules

Conrad Goodwin
20180703PRD1

Project Description

The research will focus on using specialized and unique radiological capabilities at Los Alamos National Laboratory to synthesize unprecedented organometallic compounds with actinides, including highly radioactive isotopes of neptunium, plutonium and americium. The results will open up never before possible low oxidation state chemistry for these elements and define new bonding trends. This fundamental science will be published in top journals, be internationally recognized as world leading and of direct benefit to DOE-SC programs to solve basic research needs in their Heavy Element Chemistry program. The advance in fundamental chemical bonding knowledge fosters future 'basic science knowledge-driven' innovative creative solutions to applied needs in the DOE complex aimed at tackling challenges associated with radioactive waste/chemical processing arising from used nuclear fuel (energy security), and environmental remediation problems. In addition, plutonium science is central to the national security mission of Los Alamos, and any significant new understanding in the chemistry of this element is clearly important.

Publications

Journal Articles

I. Brewster, J. T., D. N. Mangel, D. P. Saunders, H. Zafar, A. J. Gaunt, V. M. Lynch, M. A. Boreen, M. E. Garner, C. A. P. Goodwin, N. Settineri, J. Arnold and J. L. Sessler. In-plane Thorium(IV), Uranium(IV), and Neptunium(IV) Expanded Porphyrin Complexes. Submitted to *Nature Chemistry*. (LA-UR-19-28070)

Dutkiewicz, M. S., C. A. P. Goodwin, M. Perfetti, A. J. Gaunt, E. Colineau, J. Griveau, A. J. Wooles, R. G. M. Caciuffo, O. Walter and S. T. Liddle. Synthesis and Characterization of a Terminal Neptunium(V)-Mono(oxo) Complex. Submitted to *Science*. (LA-UR-21-20293)

P. Goodwin, C. A. A Synthetic Chemists' Path to High-Temperature Lanthanide Single Molecule Magnets. Submitted to *Dalton Transactions*. (LA-UR-20-22934)

P. Goodwin, C. A., A. J. Gaunt, M. T. Janicke and B. L. Scott. Autoreductive access to [AnI3(THF)4] (An = Np, Pu) for archetypal silylamide and cyclopentadienide complexes of neptunium and plutonium.. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-21-22365)

P. Goodwin, C. A., A. W. Schlimgen, T. E. Albrecht-Sch \xc3\xb6nzart, E. R. Batista, A. J. Gaunt, M. T. Janicke, S. A. Kozimor, B. L. Scott, L. M. Stevens, F. D. J. White and P. Yang. Bonding and electronic structure in soft- versus hard-donor trivalent Am and Nd imidodiphosphinate complexes. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-20-28167)

P. Goodwin, C. A., A. W. Schlimgen, T. E. Albrecht-Sch \xc3\xb6nzart, E. R. Batista, A. J. Gaunt, M. T. Janicke, S. A. Kozimor, B. L. Scott, L. M. Stevens, F. D. J. White and P. Yang. Structural and spectroscopic comparison of soft-Se vs hard-O donor bonding in trivalent americium/neodymium molecules. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-21-20831)

P. Goodwin, C. A., D. Reta and F. Ortu. Experimental and Theoretical Collaborative Work in the Field of Molecular Magnetism. Submitted to *International Journal of Quantum Chemistry*. (LA-UR-19-28416)

*P. Goodwin, C. A., F. Ortu and D. Reta. Strangely attractive: Collaboration and feedback in the field of molecular magnetism. 2020. *International Journal of Quantum Chemistry*. **120** (14): e26248. (LA-UR-20-22240 DOI: 10.1002/qua.26248)

P. Goodwin, C. A., J. Su, L. M. Stevens, F. D. J. White, T. E. Albrecht-Schonzart, E. R. Batista, J. N. Cross, W. J. Evans, A. N. Gasier, A. J. Gaunt, M. T. Janicke, T. J. Jenkins, S. A. Kozimor, I. May, B. L. Scott, J. M. Sperling, C. J. Windorff and P. Yang. Bonding and Electronic Structure in a Crystallographically Authenticated Organocalifornium Complex. Submitted to *Nature Chemistry*. (LA-UR-20-28515)

*P. Goodwin, C. A., J. Su, T. E. Albrecht-Schmitt, A. V. Blake, E. R. Batista, S. R. Daly, S. Dehnen, W. J. Evans, A. J. Gaunt, S. A. Kozimor, N. Lichtenberger, B. L. Scott and P. Yang. [Am(C Me H)]: An Organometallic Americium Complex. 2019. *Angewandte Chemie International Edition*. **58** (34): 11695-11699. (LA-UR-19-25159 DOI: 10.1002/anie.201905225)

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)

Staun, S. L., L. M. Stevens, D. E. Smiles, C. A. P. Goodwin, B. S. Billow, B. L. Scott, G. Wu, A. Tondreau, A. J. Gaunt and T. W. Hayton. Expanding the Non-aqueous Chemistry of Neptunium: Synthesis and Structural Characterization of [Np(NR2)3Cl], [Np(NR2)3Cl]1-, and [Np{N(R)(SiMe2CH2)}2(NR2)]1- (R = SiMe3). Submitted to *Inorganic Chemistry*. (LA-UR-21-21036)

Windorff, C. J., J. M. Sperling, T. E. Albrecht-Sch\xc3\xb6nzart, Z. Bai, W. J. Evans, A. N. Gaiser, A. J. Gaunt, C. A. P. Goodwin, D. E. Hobart, Z. K. Huffman, D. N. Huh, B. E. Klamm, T. N. Poe and E. Warzecha. A Single Small-Scale Plutonium Redox Reaction System Yields Three Crystallographically-Characterizable Organoplutonium Complexes. Submitted to *Inorganic Chemistry*. (LA-UR-18-29397)

*Windorff, C. J., J. M. Sperling, T. E. Albrecht-Schmitt, Z. Bai, W. J. Evans, A. N. Gaiser, A. J. Gaunt, C. A. P. Goodwin, D. E. Hobart, Z. K. Huffman, D. N. Huh, B. E. Klamm, T. N. Poe and E. Warzecha. A Single Small-Scale Plutonium Redox Reaction System Yields Three Crystallographically-Characterizable Organoplutonium Complexes. 2020. *Inorganic Chemistry*. **59** (18): 13301-13314. (LA-UR-20-23097 DOI: 10.1021/acs.inorgchem.0c01671)

Reports

P. Goodwin, C. A., J. Su, L. M. Stevens, F. D. J. White, M. T. Janicke, I. May, C. J. Windorff, J. M. Sperling, A. N. Gaiser, J. N. Cross, T. E. Albrecht-Schmitt, T. F. Jenkins, E. R. Batista, W. J. Evans, A. J. Gaunt, S. A. Kozimor, B. L. Scott and P. Yang. Bonding and Electronic Structure in a Crystallographically Authenticated Organocalifornium Complex. Unpublished report. (LA-UR-19-32441)

P. Goodwin, C. A. and A. J. Gaunt. Am–Se and Am–O imidodiphosphinate complexes. Unpublished report. (LA-UR-20-25764)

Presentation Slides

P. Goodwin, C. A. Am(III) and Ce(III) CpMe4 organometallic complexes. . (LA-UR-18-31034)

P. Goodwin, C. A. Np and Cf(III) Cp organometallic complexes. . (LA-UR-19-20947)

P. Goodwin, C. A. Cyclic voltammetry data (C23) on [Pu(tBuPyNO)4], a Pu(IV) coordination complex with a nitroxide ligand. . (LA-UR-19-21962)

P. Goodwin, C. A. [Np(DPAM)(OTMS)2] – A Np(IV) expanded porphyrin complex. . (LA-UR-19-22240)

P. Goodwin, C. A. Trans-uranic organometallic chemistry: Oxidation states, bonding and electronic. Presented at *ACS National Meeting and Expo 2019*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22542)

P. Goodwin, C. A. Pictures of drybox in 48-0001-426 to assist with repairs. . (LA-UR-19-22514)

P. Goodwin, C. A. NMR study of transition metal metallocene monoanions. . (LA-UR-19-30154)

P. Goodwin, C. A. Cyclic voltammetry data (K164) on [Np(tBuPyNO)4], a Np(IV) coordination complex with a nitroxide ligand. . (LA-UR-19-20540)

P. Goodwin, C. A. f-element Chemistry: Oxidation States, Bonding, and Electronic Structures. . (LA-UR-19-20861)

P. Goodwin, C. A. Photographs of Conrad Goodwin (Z# 328031) taken by the media office. . (LA-UR-20-21767)

P. Goodwin, C. A. DFT calculations on [VO(CpR)2]. . (LA-UR-20-22878)

P. Goodwin, C. A. Transuranium Organometallic and Soft Donor Coordination Chemistry. Presented at *Global Inorganic Discussion Weekend*, Santa Fe, New Mexico, United States, 2020-04-26 - 2020-04-26. (LA-UR-20-22939)

P. Goodwin, C. A. Transuranium Organometallic and Soft Donor Coordination Chemistry Inorganic seminar The University of Oklahoma 2nd October 2020. Presented at *Inorganic seminar*, Los Alamos, New Mexico, United States, 2020-10-02 - 2020-10-02. (LA-UR-20-27670)

P. Goodwin, C. A. EPR Spectrum of [Np(TrenTips)(Cl)]. . (LA-UR-20-28758)

P. Goodwin, C. A. Periodic Trends At The Very End – Bonding in Transuranium and Transplutonium Complexes. Presented at *Open Science Presentations*, ONLINE, New Mexico, United States, 2021-03-05 - 2021-03-05. (LA-UR-21-22086)

P. Goodwin, C. A., A. J. Gaunt and S. T. Liddle. A Np(IV)-bridged azide complex. . (LA-UR-19-29826)

P. Goodwin, C. A., M. T. Janicke, L. M. Stevens, F. D. J. White and A. J. Gaunt. F-block Seleno-imidodiphosphinate Complexes. . (LA-UR-19-32130)

P. Goodwin, C. A., S. Ciccone, W. J. Evans and A. J. Gaunt. Actinide cryptate complexes. . (LA-UR-19-30805)

P. Goodwin, C. A. and A. J. Gaunt. Voltammetry data (C35) on [Np(TrenTIPS)(Cl)], a Np(IV) coordination complex with a triamidoamine ligand. . (LA-UR-19-27163)

Murillo, J., C. A. P. Goodwin, L. M. Stevens, A. J. Gaunt and S. Fortier. ms0438 – [Np(L)(Cl)(THF)], a neptunium amide complex. . (LA-UR-21-20291)

Murillo, J., C. A. P. Goodwin, L. M. Stevens, A. J. Gaunt and S. Fortier. Murillo data. . (LA-UR-21-22354)

Staun, S. L., L. M. Stevens, C. A. P. Goodwin, A. J. Gaunt and B. L. Scott. Np cyclometallation chemistry. . (LA-UR-19-30153)

Windorff, C. J. and C. A. P. Goodwin. Actinyl phosphineoxide complexes. . (LA-UR-19-30804)

Posters

P. Goodwin, C. A., S. A. Kozimor and A. J. Gaunt. Transuranium organometallic and redox chemistry. . (LA-UR-19-25165)

New First Row Transition Metal Based Catalysts for Sustainable Energy Production

John Gordon
20180705PRD1

Project Description

While several technologies capable of generating energy exist, including nuclear, wind, solar, or hydrogen, none of these power sources alone can reasonably sustain increasing population driven energy demands in their current forms. While petroleum has long been the fuel of choice for energy production, the declining availability of light and middle cut petroleum feedstocks threatens the energy security of the nation and thus necessitates the development of novel fuel and chemical production technologies from renewable sources. The scientific results of this project will potentially provide industrially applicable techniques capable of generating transportation fuels and higher value chemicals, ameliorate possible petroleum deficits within the U.S., and provide high quality publications and potentially new Intellectual Property for the Laboratory and the DOE.

Publications

Journal Articles

Batrice, R. J., J. N. Wacker, E. N. Glass, S. Z. Jilani, Y. J. Tong, M. Nyman and K. E. Knope. Template-free cyclic hexavanadate: Synthesis, characterization, solid-state structure, and solution-state dynamics. 2019. *Polyhedron*. **169**: 266-277. (LA-UR-19-23747 DOI: 10.1016/j.poly.2019.05.014)

Presentation Slides

Batrice, R. J., P. Dub and J. C. Gordon. Outer-Sphere Ruthenium Catalysts for the Generation of Value Added Chemicals. . (LA-UR-19-31309)

Design of State-of-the-art Flow Cells for Energy Applications

Ivan Popov
20180710PRD1

Project Description

The current project is aimed to design price-competitive redox flow cells batteries that can effectively store and use greener electricity, with the overall aim of approaching the cost target on large-scale energy storage ($150/kWh) set by Department of Energy. This project is expected to discover novel electrolytes, which can be used in environmentally friendly and economically affordable redox flow cells that are critical for the national security of the United States.

Publications

Journal Articles

Andrade, G. A., I. A. Popov, C. R. Federico, P. Yang, E. R. Batista, R. Mukundan and B. L. Davis. Expanding the Potential of Redox Carriers for Flow Battery Applications. Submitted to *Journal of Materials Chemistry A*. (LA-UR-19-29590)

Bessen, N., I. A. Popov, C. Heathman, T. Grimes, P. Zalupski, L. Moreau, K. Smith, C. Booth, R. Abergel, E. R. Batista, P. Yang and J. Shafer. Lanthanide & Actinide Complexes with Aqueous Sulfur Donating Ligands. Submitted to *Inorganic Chemistry*. (LA-UR-20-27724)

Davis, B. L., G. A. Andrade, I. A. Popov, E. R. Batista, P. Yang, B. L. Scott and T. Chu. Linked Picolinamide Nickel Complexes As Charge Carriers for Non-Aqueous Flow Batteries. Submitted to *ChemSusChem*. (LA-UR-18-27470)

*Fedik, N., C. Mu, I. A. Popov, W. Wang, J. Wang, H. Wang, K. H. Bowen, A. I. Boldyrev and X. Zhang. Boron-Made N : Realization of a B\xe2\x89\xa1B Triple Bond in the B Al Cluster. 2020. *Chemistry – A European Journal*. **26** (36): 8017-8021. (LA-UR-18-24865 DOI: 10.1002/chem.202001159)

Gordon, J. C., S. Sharma, G. A. Andrade, S. Maurya, I. A. Popov, E. R. Batista, B. L. Davis, R. Mukundan, N. C. Smythe, A. Tondreau and P. Yang. Iron-iminopyridine complexes as charge carriers for non-aqueous redox flow battery applications. 2021. *Energy Storage Materials*. (LA-UR-20-28348 DOI: 10.1016/j.ensm.2021.01.035)

*Kelley, M. P., I. A. Popov, J. Jung, E. R. Batista and P. Yang. \xce\xb4 and \xcf\x86 back-donation in AnIV metallacycles. 2020. *Nature Communications*. **11** (1): 1558. (LA-UR-19-21182 DOI: 10.1038/s41467-020-15197-w)

*Liu, C., I. A. Popov, Z. Chen, A. I. Boldyrev and Z. Sun. Aromaticity and Antiaromaticity in Zintl Clusters. 2018. *Chemistry - A European Journal*. **24** (55): 14583-14597. (LA-UR-18-23061 DOI: 10.1002/chem.201801715)

*Liu, C., N. V. Tkachenko, I. A. Popov, N. Fedik, X. Min, C. Xu, J. Li, J. E. McGrady, A. I. Boldyrev and Z. Sun. Structure and Bonding in [Sb@In8Sb12]3− and [Sb@In8Sb12]5−. 2017. *Angewandte Chemie International Edition*. **58** (25): 8367-8371. (LA-UR-19-21142 DOI: 10.1002/anie.201904109)

Palmer, T. C., A. Beamer, T. A. L. Pitt, I. A. Popov, C. X. Cammack, H. D. Pratt, T. M. Anderson, E. R. Batista, P. Yang and B. L. Davis. A Comparative Review of Metal-Based Charge Carriers in Nonaqueous Flow Batteries. Submitted to *ChemSusChem*. (LA-UR-20-28027)

*Popov, I. A., B. L. Davis, R. Mukundan, E. R. Batista and P. Yang. Catalyst-Inspired Charge Carriers for High Energy Density Redox Flow Batteries. 2019. *Frontiers in Physics*. **6**. (LA-UR-18-28568 DOI: 10.3389/fphy.2018.00141)

*Popov, I. A., N. Mehio, T. Chu, B. L. Davis, R. Mukundan, P. Yang and E. R. Batista. Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. 2018. *ACS Omega*. **3** (11): 14766-14778. (LA-UR-18-22442 DOI: 10.1021/acsomega.8b01921)

*Rice, N. T., I. A. Popov, D. R. Russo, J. Bacsa, E. R. Batista, P. Yang, J. Telser and H. S. La Pierre. Design, Isolation, and Spectroscopic Analysis of a Tetravalent Terbium Complex. 2019. *Journal of the American Chemical Society*. **141** (33): 13222-13233. (LA-UR-19-26027 DOI: 10.1021/jacs.9b06622)

*Rice, N. T., I. A. Popov, D. R. Russo, T. P. Gompa, A. Ramanathan, J. Bacsa, E. R. Batista, P. Yang and H. S. La Pierre. Comparison of tetravalent cerium and terbium ions in a conserved, homoleptic imidophosphorane ligand field. 2020. *Chemical Science*. **11** (24): 6149-6159. (LA-UR-20-22218 DOI: 10.1039/D0SC01414A)

Tkachenko, N. V., I. A. Popov, A. Mu\xc3\xb1oz-Castro, Z. M. Sun and A. I. Boldyrev. Bridging Aromatic/Antiaromatic Units. Recent Advances in Aromaticity and Antiaromaticity in Main-group and Transition-metal clusters.. Submitted

to *European Journal of Inorganic Chemistry*. (LA-UR-20-27965)

Xu, H., I. A. Popov, N. V. Tkachenko, Z. Wang, A. I. Boldyrev and Z. M. Sun. \xcf\x83-Aromaticity-Induced Stabilization of Heterometallic Supertetrahedral Clusters [Zn6Ge16]4– and [Cd6Ge16]4–. 2020. *Angewandte Chemie*. **132** (39): 17439-17443. (LA-UR-20-24262 DOI: 10.1002/ange.202008276)

Xu, Y., N. V. Tkachenko, L. Qiao, I. A. Popov, A. Mu\xc3\xb1oz-Castro, A. I. Boldyrev and Z. M. Sun. Ternary Aromatic and Anti-aromatic Clusters Stemmed from a hypho-Zintl Precursor [Sn2Sb5]3-. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-20-28353)

*Zhang, X., I. A. Popov, K. A. Lundell, H. Wang, C. Mu, W. Wang, H. Schn\xc3\xb6ckel, A. I. Boldyrev and K. H. Bowen. Realization of an Al\xe2\x89\xa1Al Triple Bond in the Gas-Phase Na Al Cluster via Double Electronic Transmutation. 2018. *Angewandte Chemie International Edition*. **57** (43): 14060-14064. (LA-UR-18-22726 DOI: 10.1002/anie.201806917)

Presentation Slides

Popov, I. A. Ligand Effects on the Multi-Electron Redox Properties of Fe Complexes. Presented at *256th ACS National Meeting*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-28005)

Popov, I. A., M. P. Kelley, E. R. Batista and P. Yang. Importance of the unprecedented \xce\xb4 back-donation in AnIV metallacycles. Presented at *256th ACS National Meeting*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-27949)

Popov, I. A., M. P. Kelley, E. R. Batista and P. Yang. \xce\xb4 Back-Donation in AnIV Metallacycles (An=Th, Pa, U, Np, Pu). Presented at *Plutonium Futures 2018*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28566)

Posters

Popov, I. A., T. Chu, G. A. Andrade, S. Maurya, B. L. Scott, B. L. Davis, R. Mukundan, E. R. Batista and P. Yang. Theoretical Modeling of Charge Carriers for High Energy Density Redox Flow Batteries. Presented at *Workshop on Non-Aqueous Flow Batteries*, Santa Fe, New Mexico, United States, 2019-01-30 - 2019-01-31. (LA-UR-19-20645)

Investigating Actinide-Based Molecular Magnetism with Electron Paramagnetic Resonance

Benjamin Stein
20180759PRD4

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).

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)

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)

Enabling Artificial Selection Programs through Characterizing the Lifecycle of Green Algae

Shawn Starkenburg
20190616PRD1

Project Description

Characterizing the life cycle of Scenedesmus obliquus, a candidate feedstock for biofuel production, would enable artificial selection programs for desired algal traits. Artificial selection programs have the potential to dramatically increase the productivity of algal-based renewable energy feedstocks. This new area of research complements the existing bioenergy portfolio of Los Alamos National Laboratory and directly aligns with Los Alamos' mission to provide energy independence and security solutions for the nation.

Publications

Journal Articles

Hanschen, E. R., B. Hovde and S. R. Starkenburg. Evaluating the quality of algal genome assemblies. Submitted to *Algal Research*. (LA-UR-20-22201)

Hanschen, E. R. and S. R. Starkenburg. The state of algal genomics. Submitted to *Algal Research*. (LA-UR-20-21021)

*Hovde, B. T., H. E. Daligault, E. R. Hanschen, Y. A. Kunde, M. B. Johnson, S. R. Starkenburg and S. L. Johnson. Detection of Abrin-Like and Prepropulchellin-Like Toxin Genes and Transcripts Using Whole Genome Sequencing and Full-Length Transcript Sequencing of Abrus precatorius. 2019. *Toxins*. **11** (12): 691. (LA-UR-19-27275 DOI: 10.3390/toxins11120691)

Schambach, J. Y., A. M. Finck, P. Kitin, C. G. Hunt, E. R. Hanschen, B. Vogler, S. R. Starkenburg and A. N. Barry. Growth, total lipid, and omega-3 fatty acid production by Nannochloropsis spp. cultivated with raw plant substrate. 2020. *Algal Research*. **51**: 102041. (LA-UR-20-23298 DOI: 10.1016/j.algal.2020.102041)

Presentation Slides

Hanschen, E. R. The state of algal genomics: quality and diversity. Presented at *Algal Biomass Organization*, Online, New Mexico, United States, 2020-08-12 - 2020-09-30. (LA-UR-20-26722)

Hanschen, E. R., S. R. Starkenburg, K. K. Hixson, M. Costa, S. Moinuddin, K. Engbrecht, T. Fillmore, R. Sayre, M. S. Lipton, D. T. Hanson, O. Monje, J. Richards, L. Davin and N. Lewis. Patterns of gene expression in Arabidopsis thaliana in response to microgravitational environment. Presented at *American Society for Gravitational and Space Research*, Denver, Colorado, United States, 2019-11-20 - 2019-11-23. (LA-UR-19-31557)

Posters

N. Abbott, A. R., E. R. Hanschen and S. R. Starkenburg. Environmental conditions causing mating of green alga Scenedesmus. Presented at *Student Symposium 2019*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27334)

Hanschen, E. R., J. E. W. Polle, J. Umen and S. R. Starkenburg. Sexual reproduction and mating in the green alga Scenedesmus obliquus. Presented at *Sequencing, Finishing, and Analysis in the Future*, Sante Fe, New Mexico, United States, 2019-05-21 - 2019-05-23. (LA-UR-19-24631)

Multiscale Quantitative Description of Drug Resistance Mechanisms in Bacterial Systems

Sandrasegaram Gnanakaran
20190644PRD3

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.

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)

Toward a Universal Description for Aqueous Solutions

Alp Findikoglu
20190653PRD4

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.

Publications

Journal Articles

*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. 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., 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)

Forecasting Valley Fever Disease Risk Using Machine Learning

Carrie Manore
20200682PRD1

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

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. Submitted to *Health Policy OPEN*. (LA-UR-20-30424)

Gorris, M. E., S. Anenberg, D. Goldberg, G. Kerr, J. Stowell, D. Tong and B. Zaitchik. Shaping the future of science: COVID-19 highlighting the importance of GeoHealth. Submitted to *GeoHealth*. (LA-UR-21-21425)

Keyel, A. C., M. E. Gorris, I. Rochlin, J. A. Uelman, 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 and R. L. Smith. A qualitative evaluation of West Nile virus models and their application to local public health decision-making. Submitted to *PLOS Neglected Tropical Diseases*. (LA-UR-21-22349)

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)

Presentation Slides

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)

Geochemical-Geomechanical Feedback in Stressed Fracture Systems

James Carey
20200769PRD3

Project Description

This research on fracture properties in the subsurface addresses national energy security. Fractures control access to hydrocarbons (unconventional shale gas), development of geothermal energy, long-term storage of pollutants (underground waste disposal; carbon dioxide (CO_2) sequestration), and nuclear waste repository security. This project explores how chemical reactions interact with fractures and faults to predict fluid flow through fractures in the subsurface. If successful, the project will produce previously unavailable experimental results using unique Los Alamos National Laboratory-developed equipment to allow predictions of the evolution of the permeability of subsurface fracture systems. Subsurface fractures have significant impacts to the performance of numerous Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions, including containment of nuclear explosions; production of hydrocarbons; long-term sequestration of CO_2; geothermal energy; and nuclear waste disposal.

Impacts of Climate and Land Use on Global River Dynamics

Jonathan Schwenk
20170668PRD1

Project Description

By using global datasets of remotely sensed imagery to quantify river dynamics, this project will directly improve our ability to predict and mitigate risks to infrastructure, agriculture, and navigation due to changing channels. Rivers and floodplains play an essential role in the storage and transport of water sediment and biogeochemical constituents. Quantifying the magnitude and controls on these fluxes and impacts to infrastructure helps support DOE science missions and the NNSA's national security missions. An improved predictive understanding of river responses to floods and droughts will aid in disaster planning and assessing risk to critical infrastructure.

Technical Outcomes

This project resulted in three software packages (RivGraph, rivmask, and RaBPro), architecture for acquiring, standardizing, and exploiting global geospatial data, and algorithmic advancements aimed at feature detection via machine learning. We also developed a first-generation global model to predict riverbank erosion rates based on easily measurable watershed characteristics.

Publications

Journal Articles

*Gran, K. B., C. Dolph, A. Baker, M. Bevis, S. J. Cho, J. A. Czuba, B. Dalzell, M. Danesh-Yazdi, A. T. Hansen, S. Kelly, Z. Lang, J. Schwenk, P. Belmont, J. C. Finlay, P. Kumar, S. Rabotyagov, G. Roehrig, P. Wilcock and E. Foufoula-Georgiou. The Power of Environmental Observatories for Advancing Multidisciplinary Research, Outreach, and Decision Support: The Case of the Minnesota River Basin. 2019. *Water Resources Research*. **55** (4): 3576-3592. (LA-UR-18-29803 DOI: 10.1029/2018WR024211)

Rowland, J. C., J. P. Schwenk, J. Muss, E. Shelef, S. Stauffer and D. Ahrens. Permafrost limits river bank erosion in the Arctic but size matters. Submitted to *Nature Geoscience*. (LA-UR-20-22915)

*Schwenk, J. P., A. Piliouras and J. C. Rowland. Determining flow directions in river channel networks using planform morphology and topology. 2020. *Remote Sensing of Environment*. **8** (1): 87-102. (LA-UR-19-22689 DOI: 10.5194/esurf-8-87-2020)

*Vulis, L., A. Tejedor, J. P. Schwenk, A. Piliouras, J. C. Rowland and E. Foufoula-Georgiou. Channel Network Control on Seasonal Lake Area Dynamics in Arctic Deltas. 2020. *Geophysical Research Letters*. **47** (7): e2019GL086710. (LA-UR-19-32740 DOI: 10.1029/2019GL086710)

Presentation Slides

Schwenk, J. P., A. Piliouras, Y. Zhang, M. M. Fratkin, J. C. Rowland, M. M. Douglas, A. Chadwick and M. P. Lamb. Permafrost control on river migration along the Koyukuk River, AK. Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32556)

Posters

Schwenk, J. P., J. C. Rowland, A. Piliouras, A. Tejedor and E. Foufoula-Georgiou. Automatic Extraction of Channel Network Topology. Presented at *American Geophysical Union*, Washington, D.C., District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31483)

Other

Schwenk, J. P., J. C. Rowland and A. Piliouras. Readme for data from Determining flow directions in river channel networks using planform morphology and topology. Dataset. (LA-UR-19-23211)

Developing a Unique Technology to Control Emerging Threats of Antibiotic-resistant Pathogens

Anand Kumar
20170671PRD2

Project Description

The project goal is to control C. difficile infections (CDI), their re-occurrence, and the rise of antibiotic resistance. C. difficile infections pose threats to our nation's public health and security. Our proposed work takes a systematic approach to utilize the normal human gut flora to naturally control CDI and antibiotic resistance.

Technical Outcomes

This project has successfully integrated a combination of techniques, including microfluidics, culturing, flow sorting, isolation and sequencing, to develop a 'High-Throughput Microbiome Screening' (HTMS) platform. The team has utilized this developed HTMS platform to identify therapeutic bacterial species from a healthy human skin microbiome that naturally inhibit methicillin-resistant Staphylococcus aureus, MRSA.

Publications

Journal Articles

Arruda, A. G., L. Deblais, V. Hale, M. Pairis-Garcia, V. Srivastava, D. Kathayat, A. Kumar and G. Rajashekara. A cross-sectional study of the nasal and fecal microbiota of sows from different health status within six commercial swine farms. Submitted to *PeerJ*. (LA-UR-20-28622)

Presentation Slides

Kumar, A. Targeting Emerging Pathogen Infections with Next Generation Therapeutic Probiotics. Presented at *MICROBIOME & PROBIOTICS SERIES: USA*, San Diego, California, United States, 2019-10-29 - 2019-10-30. (LA-UR-19-31051)

Posters

Kumar, A., K. Martinez, M. R. Kron, J. M. Kelliher, B. M. Butler, J. L. Aslin, S. E. Pasqualoni, A. E. K. Dichosa and P. S. G. Chain. Combating antibiotic-resistant pathogens by microbiome-based therapeutics. Presented at *2019 Chemical and Biological Defense Science & Technology (CBD S&T) Conference*, Cinncinati, Ohio, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-31339)

Forecasting Failure

Bertrand Rouet-Leduc
20170673PRD2

Project Description

A large earthquake in Cascadia or California would devastate the regional and potentially national economies. The primary national security challenge this project will address is attempting to characterize when a large earthquake may occur and how large it may be so that preparatory action may be taken. Our secondary security challenge is applying this same technology to anthropogenically induced seismicity, particularly in the Midwest. Can we tell when a large, human induced earthquake will take place and how large it will be, so that we can take action to prevent it? That is the secondary goal. The novelty of our work is the use of machine learning to discover and understand new physics of failure, through examination of the full continuous time signal. The future of earthquake physics will rely heavily on machine learning to process massive amounts of raw seismic data. Our work represents an important step in this direction. The outcomes of this project are expected to have broad technical application. Not only does it have import to earthquake forecasting, but also the approach is far-reaching, applicable to potentially all failure scenarios including nondestructive testing, brittle failure of all kinds, avalanche, etc.

Technical Outcomes

This project built a machine learning framework for the analysis of seismic data, by relating features of the seismic data to bulk properties of faults. The team applied this framework to tectonic tremor and found features of the seismic data to track geodetic displacement in Cascadia. In parallel, the team developed a machine learning framework to analyze Interferometric Synthetic Aperture Radar (InSAR) time series, enabling us to detect minute deformation on faults with far greater precision than the state-of-the-art.

Publications

Journal Articles

Hulbert, C. L. Estimating the Physical State of a Laboratory Slow Slipping Fault from Seismic Signals. Submitted to *Nature Geoscience, ArXiv*. (LA-UR-18-20487)

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)

G. Rouet-Leduc, B. P., C. L. Hulbert and P. A. Johnson. Breaking Cascadia's Silence: Machine Learning Reveals the Constant Chatter of the Megathrust. Submitted to *Arxiv; Nature*. (LA-UR-18-24744)

G. Rouet-Leduc, B. P., P. A. Johnson and C. L. Hulbert. Breaking Cascadia's Silence: Machine Learning Reveals the Constant Chatter of the Megathrust. Submitted to *arXiv:1805.06689 [physics.geo-ph] (2018)*. (LA-UR-18-29847)

*Rouet-Leduc, B., C. Hulbert, D. C. Bolton, C. X. Ren, J. Riviere, C. Marone, R. A. Guyer and P. A. Johnson. Estimating Fault Friction From Seismic Signals in the Laboratory. 2018. *Geophysical Research Letters*. **45** (3): 1321-1329. (LA-UR-17-29312 DOI: 10.1002/2017GL076708)

*Rouet-Leduc, B., C. Hulbert, I. W. McBrearty and P. A. Johnson. Probing Slow Earthquakes With Deep Learning. 2020. *Geophysical Research Letters*. **47** (4). (LA-UR-19-27444 DOI: 10.1029/2019GL085870)

Rouet-Leduc, B., C. Hulbert, N. Lubbers, K. Barros, C. J. Humphreys and P. A. Johnson. Machine Learning Predicts Laboratory Earthquakes. 2017. *Geophysical Research Letters*. **44** (18): 9276-9282. (LA-UR-16-26108 DOI: 10.1002/2017GL074677)

Posters

Johnson, P. A., A. A. Delorey, K. M. Barros, N. E. Lubbers, B. P. G. Rouet-Leduc and C. L. Hulbert. Machine Learning algorithm predicts time to failure of laboratory earthquake machine. . (LA-UR-17-23157)

Prediction of Magnetic Properties of Actinide Complexes Using Ab Initio Methods

Julie Jung
20170677PRD2

Project Description

The U.S. National Energy Policy states the critical need for the expansion of nuclear energy to enhance energy security and reduce domestic dependence on foreign fossil fuels. Yet, comprehensive and innovative storage or reprocessing solutions hinge on physics and chemistry knowledge going far beyond what is currently available. Separation of the highly hazardous minor actinides from the rest of the waste would greatly facilitate disposal by drastically reducing the storage time of bulk waste and the volume of waste required for long-term storage. Unfortunately, due to the similarities between minor actinides and lanthanides, a procedure to isolate these elements is still missing. This work is the first systematic study of the magnetic properties of actinide molecular systems, which will enable us to draw structure/property correlations. This will not only improve our understanding of the subtle differences in the chemistry in transuranium elements, it will also help us identify, and potentially design, new molecular species capable of effecting the separation of minor actinides. The impact of having this predictability will advance us towards cleaner and more cost-effective reprocessing mechanisms to deal with spent nuclear fuel, which addresses Los Alamos missions in plutonium excellence, energy security, repository science, and long-term waste management.

Technical Outcomes

Using a unique combination of first principle simulations and magnetic measurements, molecular systems containing actinide ions were systematically studied. New structure-property correlations were established, showing how structural and chemical feature influence the nature and strength of metal-ligand interactions. This work brings us a step closer from being able to selectively extract the minor actinides from spent nuclear fuel, and hence, make nuclear energy and waste management more efficient and sustainable.

Publications

Journal Articles

*Autillo, M., M. A. Islam, J. Jung, J. Pilm\xc3\xa9, N. Galland, L. Guerin, P. Moisy, C. Berthon, C. Tamain and H. Bolvin. Crystallographic Structure and Crystal Field Parameters in the [AnIV(DPA)3]2 – series, An= Th, U, Np, Pu. 2020. *Physical Chemistry Chemical Physics*. **22** (25): 14293-14308. (LA-UR-20-23294 DOI: 10.1039/D0CP02137G)

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Presentation Slides

A. O. Jung, J. C. Understanding Actinide Bonding with High Accuracy. . (LA-UR-18-24995)

A. O. Jung, J. C. Using effective models to “translate” ab initio energies and wave functions\xe2\x80\xa8 into physics and chemistry. . (LA-UR-19-31270)

A. O. Jung, J. C., H. Bolvin, M. A. Islam and C. Berthon. Ab initio Derivation of Crystal Field Parameters in Lanthanide Series. Presented at *European Conference on Molecular Magnetism*, Florence, Italy, 2019-09-15 - 2019-09-18. (LA-UR-19-28551)

A. O. Jung, J. C., P. Yang and E. R. Batista. First principle simulation of the EPR g-values in actinide complexes (to support chemical bonding analysis). Presented at *4th International Workshop on Advanced Techniques in Actinide Spectroscopy*, NICE, France, 2018-11-06 - 2018-11-09. (LA-UR-18-30275)

Posters

A. O. Jung, J. C. Understanding metal-ligand bonding in actinide complexes with high accuracy. . (LA-UR-18-24861)

A. O. Jung, J. C. Bacteria-inspired Energy Production: Insight from Quantum Chemistry. . (LA-UR-19-28508)

A. O. Jung, J. C., P. Yang, E. R. Batista and S. A. Kozimor. Computational Chemistry: \xe2\x80\xa8A Powerful Tool to Analyze Actinide Molecules !. . (LA-UR-18-28017)

A. O. Jung, J. C., P. Yang, E. R. Batista and S. A. Kozimor. Computational Chemistry: \xe2\x80\xa8A Powerful Tool to Analyze Actinide Molecules !. . (LA-UR-18-28127)

A. O. Jung, J. C., P. Yang and E. R. Batista. Electronic Structure and Optical Spectroscopy of Actinide Complexes Using Correlated Multi-Reference Calculations. Presented at *2018 Conference on Excited States Processes*, SANTA FE, New Mexico, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-24807)

Epigenetic Control of Synchronized Proliferation in Harmful Algal Blooms (HABs)

Babetta Marrone
20170690PRD4

Project Description

The increased frequency of harmful algal blooms in regions in the United States affected by climate change has produced heightened scientific and regulatory attention; these blooms, by destroying the environment, cause economic instability, potential political unrest, and significant health issues. Research has focused on identifying harmful algal species and creating bloom prediction models; however, to date, little is known about the molecular and cellular physiology of these blooms. This knowledge is critical for predicting, suppressing, and controlling these deleterious events. The proposed research identifies important epigenetic processes that regulate harmful algal bloom formation and provides greater insight into critical mechanisms of action that could be harnessed to mitigate harmful algal blooms in coastal waters for increased regional and global security. Harmful algal blooms impact human health and economic stability as they ruin water quality, impact food safety, induce sickness and death from toxin exposure, and cause biothreats. Understanding regulation of harmful algal blooms directly contributes to program needs for the Department of Homeland Security (global security of bio-toxin production), the Department of Defense (sailor health and port environmental impacts), and the Department of Energy (bioenergy and environmental climate impacts).

Technical Outcomes

This project successfully cultivated a harmful algae bloom (HAB) species in vitro and recapitulated its bloom phenotype. These laboratory cultivation capabilities were established in conjunction with high throughput assessments of cellular functions and characteristics, including assays for measuring epigenetic regulation of algae genomes. DNA methylation assessment revealed that epigenetic mechanisms control microalgae behavior and phenotype. By harnessing these capabilities and manipulating the epigenome, we can develop novel strategies to manage HABs for biosecurity purposes.

Publications

Journal Articles

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*Tyler, C. R., S. Noor, T. L. Young, V. Rivero, B. Sanchez, S. Lucas, K. K. Caldwell, E. D. Milligan and M. J. Campen. Aging Exacerbates Neuroinflammatory Outcomes Induced by Acute Ozone Exposure. 2018. *Toxicological Sciences*. **163** (1): 123-139. (LA-UR-18-20155 DOI: 10.1093/toxsci/kfy014)

Zychowski, K. E., C. R. Steadman, B. Sanchez, M. Harmon, J. Liu, H. Irshad, J. McDonald, B. Bleske and M. J. Campen. Vehicular Particulate Matter (PM) Characteristics Impact Vascular Outcomes Following Inhalation. Submitted to *Toxicology and Applied Pharmacology*. (LA-UR-19-22500)

*Zychowski, K. E., V. Kodali, M. Harmon, C. R. Tyler, B. Sanchez, Y. Ordonez Suarez, G. Herbert, A. Wheeler, S. Avasarala, J. M. Cerrato, N. K. Kunda, P. Muttil, C. Shuey, A. Brearley, A. Ali, Y. Lin, M. Shoeb, A. Erdely and M. J. Campen. Respirable Uranyl-Vanadate-Containing Particulate Matter Derived From a Legacy Uranium Mine Site Exhibits Potentiated Cardiopulmonary Toxicity. 2018. *Toxicological Sciences*. **164** (1): 101-114. (LA-UR-18-21620 DOI: 10.1093/toxsci/kfy064)

Machine Learning the Physics of an Active Gold Mine

Daniel Trugman
20180700PRD1

Project Description

This work will address energy security and national security. Our work will advance earthquake forecasting, including human induced earthquakes. For instance, the energy storage site at Cushing Oklahoma is located in a highly earthquake-active region due to wastewater injection. This work will better predict if an earthquake near Cushing is imminent. In addition, it will tell us if a large tectonic quake is approaching, for instance in the Cascadia region. The high-level goals of this work are to advance our understanding of Earth faults and advance earthquake forecasting. This work will impact DOE/NNSA national security missions. For instance, a megaquake in Cascadia will have dramatic impact on the regional and national economy. A quake at Cushing, has the potential to disturb oil reserves or their distribution, and could have a negative impact on the national economy.

Technical Outcomes

Understanding how earthquakes get started is a fundamental research question in seismology that has important implications for natural hazards and critical infrastructure. This project advanced new techniques to analyze large waveform datasets to better understand the earthquake nucleation process. Notable technical achievements of this project include the development of improved algorithms for earthquake early warning, leveraging high-performance computing resources to detect small foreshock earthquakes, and a detailed analysis of the 2019 Ridgecrest, California earthquake sequence.

Publications

Journal Articles

*Kong, Q., D. T. Trugman, Z. E. Ross, M. J. Bianco, B. J. Meade and P. Gerstoft. Machine Learning in Seismology: Turning Data into Insights. 2019. *Seismological Research Letters*. **90** (1): 3-14. (LA-UR-18-28089 DOI: 10.1785/0220180259)

*Koper, K. D., K. L. Pankow, J. C. Pechmann, J. M. Hale, R. Burlacu, W. L. Yeck, H. M. Benz, R. B. Herrmann, D. T. Trugman and P. M. Shearer. Afterslip Enhanced Aftershock Activity During the 2017 Earthquake Sequence Near Sulphur Peak, Idaho. 2018. *Geophysical Research Letters*. **45** (11): 5352-5361. (LA-UR-18-22721 DOI: 10.1029/2018GL078196)

*Qin, Y., X. Chen, J. I. Walter, J. Haffener, D. T. Trugman, B. M. Carpenter, M. Weingarten and F. Kolawole. Deciphering the Stress State of Seismogenic Faults in Oklahoma and Southern Kansas Based on an Improved Stress Map. 2019. *Journal of Geophysical Research: Solid Earth*. **124** (12): 12920-12934. (LA-UR-18-27043 DOI: 10.1029/2019JB018377)

*Ross, Z. E., D. T. Trugman, E. Hauksson and P. M. Shearer. Searching for hidden earthquakes in Southern California. 2019. *Science*. **364** (6442): 767-771. (LA-UR-19-20273 DOI: 10.1126/science.aaw6888)

*Ross, Z. E., D. T. Trugman, K. Azizzadenesheli and A. Anandkumar. Directivity Modes of Earthquake Populations with Unsupervised Learning. 2020. *Journal of Geophysical Research: Solid Earth*. **125** (2): e2019JB018299. (LA-UR-19-26206 DOI: 10.1029/2019JB018299)

*Ross, Z. E., E. S. Cochran, D. T. Trugman and J. D. Smith. 3D fault architecture controls the dynamism of earthquake swarms. 2020. *Science*. **368** (6497): 1357-1361. (LA-UR-20-20957 DOI: 10.1126/science.abb0779)

*Shearer, P. M., R. E. Abercrombie, D. T. Trugman and W. Wang. Comparing EGF Methods for Estimating Corner Frequency and Stress Drop From Wave Spectra. 2019. *Journal of Geophysical Research: Solid Earth*. **124** (4): 3966-3986. (LA-UR-18-30681 DOI: 10.1029/2018JB016957)

*Trugman, D. T. Stress-Drop and Source Scaling of the 2019 Ridgecrest, California, Earthquake Sequence. 2020. *Bulletin of the Seismological Society of America*. **110** (4): 1859-1871. (LA-UR-20-20288 DOI: 10.1785/0120200009)

Trugman, D. T., G. C. Beroza and P. A. Johnson. Machine Learning in Geoscience: Riding a Wave of Progress. 2019. *Eos*. **100**. (LA-UR-19-22852 DOI: 10.1029/2019EO122671)

Trugman, D. T., I. McBrearty, C. Bolton, R. A. Guyer, C. Marone and P. A. Johnson. The Spatio-temporal Evolution of Granular Microslip Precursors to Laboratory Earthquakes. Submitted to *Geophysical Research Letters*. (LA-UR-20-22864)

*Trugman, D. T., M. T. Page, S. E. Minson and E. S. Cochran. Peak Ground Displacement Saturates Exactly When Expected: Implications for Earthquake Early Warning. 2019. *Journal of Geophysical Research: Solid Earth*. 2018JB017093. (LA-UR-18-30809 DOI: 10.1029/2018JB017093)

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Trugman, D. T. and P. M. Shearer. Strong Correlation between Stress Drop and Peak Ground Acceleration for Recent M \xc2\xa01–4 Earthquakes in the San Francisco Bay Area. 2018. *Bulletin of the Seismological Society of America*. (LA-UR-18-20708 DOI: 10.1785/0120170245)

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Presentation Slides

Trugman, D. T. Machine Learning Applications to Earthquake Source Characterization and Hazard Analysis. . (LA-UR-18-24892)

Trugman, D. T. Do large and small earthquakes start alike? Rupture determinism and earthquake early warning. . (LA-UR-19-20107)

Trugman, D. T. Unsupervised Learning : A Gentle Introduction. Clustering the ComCat Earthquake Catalog using Python’s Scikit-Learn Package.. Presented at *Seismological Society of America*, Seattle, Washington, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23604)

Trugman, D. T. Big Data, Small Earthquakes. . (LA-UR-19-24388)

Trugman, D. T. Earthquake Nucleation: Observations and Applications From Megaquakes in Japan to Microforeshocks in California. . (LA-UR-19-27171)

Trugman, D. T. New Perspectives on Earthquake Nucleation from Megaquakes in Japan and Microforeshocks in California. . (LA-UR-19-29868)

Posters

Trugman, D. T., Z. E. Ross and P. A. Johnson. Anti-similar aftershocks in the Ridgecrest, California earthquake sequence. Presented at *Southern California Earthquake Center Annual Meeting*, Palm Springs, California, United States, 2019-09-09 - 2019-09-09. (LA-UR-19-28255)

Principles for Optimal Establishment and Resilience of Microbial Communities

Michaeline Albright
20180746PRD3

Project Description

Deciphering fundamental principles of microbial invasion will raise the probability of successfully engineering microbial communities for applications to address a number of national security challenges. For example, robust understanding of principles of microbial invasion will allow for 1) effective development and deployment of probiotics for soldier health 2) improvements in agricultural soil microbe manipulations for increased food and energy security and 3) remediation and restoration of degraded environments for climate impact management.

Technical Outcomes

The project developed an innovative test system. Instead of examining single invasion events, our system enabled analysis of hundreds of simultaneous events. With this system, the team showed that microbiome engineering strategies can be prioritized. This work emphasized binning microbiome engineering strategies into a few conceptual categories and demonstrating that the impact of the conceptual categories on invasion success can be ranked, dependent on organism type (i.e., bacteria versus fungi) and environment type.

Publications

Journal Articles

N. Albright, M. B., S. A. Sevanto and J. M. Dunbar. Biotic Interactions Are More Important than Propagule Pressure in Microbial Community Invasions. 2020. *mBio*. **11** (5): e02089-20. (LA-UR-19-27879 DOI: 10.1128/mBio.02089-20)

N. Albright, M. B., S. Louca, D. Winkler, K. L. Feeser, S. Haig, K. Whiteson, J. Emerson and J. M. Dunbar. Solutions in Microbiome Engineering: Prioritizing Barriers to Organism Establishment. Submitted to *ISME Journal*. (LA-UR-20-30490)

Presentation Slides

N. Albright, M. B. Impacts of Microbial Invasions on Community Assembly and Ecosystem Functioning in Natural and Engineered Systems. . (LA-UR-21-21512)

N. Albright, M. B. and J. M. Dunbar. Principles for Engineering Microbial Composition and Ecosystem Functioning. Presented at *Applied and Environmental Microbiology Gordon Research Conference*, South Hadley, Massachusetts, United States, 2019-07-13 - 2019-07-19. (LA-UR-19-26384)

Posters

N. Albright, M. B., L. A. Gallegos-Graves, J. C. Thompson, R. Johansen, D. Ulrich, K. L. Avery, B. Timalsina, K. K. Stringfield, A. C. Runde, D. L. Lopez, T. M. Yoshida, M. Shakya, S. A. Sevanto and J. M. Dunbar. Principles for Microbiome Engineering. . (LA-UR-19-28938)

High Efficiency Automated Leaching of Gloveboxes (HEAL-GB)

Benjamin Karmiol
20190524MFR

Project Description

There are many legacy gloveboxes (GB) that require decommissioning. In particular, many Los Alamos gloveboxes will need to be replaced to meet the increased Laboratory pit production goals for national security. Additionally Plutonium-238 heat source production will increase. Safe and efficient decontamination for decommissioning activities and to meet Pu-238 heat source production goals will be a challenge and requires further research and development. This project will deliver the data and technology needed to develop a process scale High Efficiency Automated Leaching of Gloveboxes (HEAL-GB) system. This system will allow for easier/less expensive GB disposal and/or Pu-238 cladding decontamination , less waste, lower dose rates and less risk of injury. The end-goal is to fully automate the process using a robotic arm. This project will focus on understanding the effect of parameters such as concentration, duration, temperature and mixing on system performance. The expected outcome is data that will provide the information necessary to scale-up the system.

Technical Outcomes

Successful development and testing of several synergistic technologies led to an integrated electrochemical decontamination system for glove boxes. In addition, a system for decontaminating plutonium (Pu)-238 heat source cladding was also successfully designed and tested. The glove box system includes a high performance elctrochemical cell, a suction head delivery system, a novel contactor for actinide removal, an online measurement system to ensure sufficient oxidizing ion concentration, and an acoustic measurement system for thickness monitoring.

Publications

Presentation Slides

Karmiol, B. Electrochemical Decontamination Development Summary - Potential for Collaborations. . (LA-CP-20-20635)

Karmiol, B., J. T. Stritzinger, D. A. T. Rodriguez, S. P. Walsh, M. J. Monreal, J. J. Monroe, N. Xu and S. D. Mckee. Electrochemical approach to metal decontamination. Presented at *2019 Southwest-Rocky Mountain Regional Meeting of the American Chemical Society*, El Paso, Texas, United States, 2019-11-13 - 2019-11-15. (LA-UR-19-31321)

T. Rodriguez, D. A., B. Karmiol, J. T. Stritzinger, S. P. Walsh, M. J. Monreal, K. R. Weisbrod and J. J. Monroe. High Efficiency Automated Leaching of Glove Boxes. Presented at *JOWOG 22-2*, Los Alamos, New Mexico, United States, 2019-07-15 - 2019-07-15. (LA-UR-19-27535)

Glovebox Diagnostics to Support Plutonium Cleaning Operations

Daniel Kelly
20200470MFR

Project Description

This work will support the national security challenge of maintaining a robust and cost-efficient Pit Manufacturing program at Los Alamos National Laboratory. The goals of the work are to develop diagnostics to assess the chemical integrity of fluids used for cleaning, machining, and density measurements during pit manufacturing. Further the work aims to develop compact and robust technology which can be deployed within a glovebox and used for real-time measurements during manufacturing. The diagnostics would interrogate the chemical integrity of cleaning fluids, allowing for their efficacy to be assessed based on prior benchtop cleaning studies. This knowledge reduces uncertainty in cleaning efficiency, reduces process downtime for unnecessary fluid changes, reduces waste volumes, and potentially reduces worker rad exposure. The expected outcome of Phase 1 work is the successful proof on concept to using infrared and optical spectroscopies to chemically characterize manufacturing fluids, and to begin the transition of this technology into the manufacturing line. Phase 2 work will upgrade cleaning processes to industry standards in vapor degreasing, and will study new cleaning fluids for use in pit manufacturing to circumvent future environmental compliance concerns.

Technical Outcomes

This project has shown that it is feasible to use a handheld Fourier Transform Infrared Spectrometer within a glovebox, to determine the identity and quality of fluids used in Pit Manufacturing processes. This work has also shown that this instrument has the capability to measure the cleanliness of solid surface within the processing line. Correlations between fluid quality and surface cleanliness can be made to determine the likelihood of downstream processing steps after part cleaning.

Revolutionary Separations for Efficient and Cost-Effective Americium-241 Production

George Goff
20200496MFR

Project Description

The need to shrink the aqueous processing footprint at the Los Alamos Plutonium Facility (PF-4) has been clearly identified as a prerequisite towards achieving the nationally important 30 Pits per Year production mission. This project will perform vital research & development on new separation equipment developed by the Laboratory, with the hypothesis that simultaneous purification of plutonium (Pu) and recovery of Americium-241 may be possible in the same piece of process equipment. This project will investigate parameters and potential adaptations. A successful project will significantly decrease the aqueous processing footprint, shorten the batch processing time, and reduce the effective dose to workers.

Technical Outcomes

This project successfully adapted the chemistry used in the extraction chromatography purification of Americium-241 (ion exchange) and demonstrated the feasibility of implementing this chemistry in an advanced liquid-liquid contactor. This liquid-liquid process shows faster processing times than the conventional technology with a smaller footprint. Testing with rare earth surrogates indicated comparable or higher separation factors.

A Multidisciplinary Approach to Advance Our Understanding of Actinide-Bearing Molten Salt Systems

Marisa Monreal
20190650DI

Project Description

The national security challenges this project addresses are Energy Security and Stockpile Stewardship. The high-level goal of this research is to couple innovative physical and chemical property measurements with modeling and simulation towards a better understanding of actinide-bearing molten salt systems. The expected outcomes of this project are an advancement of the science and engineering that underpins engineered molten salt systems, via the development of techniques that will be enduring with respect to both experiment and theoretical examination of complex molten salt systems. This research will have high impact on the 30+ Pits Per Year (PPY) manufacturing mission (i.e., uranium and plutonium metal purification), as well as on the Nuclear Energy missions across the complex (e.g., reactor development, spent fuel reprocessing, nonproliferation, safeguards).

Technical Outcomes

Multiple unique new actinide-molten salt capabilities were established and used to collect thermophysical property, chemical property, and modeling and simulation data. These capabilities were successfully integrated, and new insights were gained into these systems.

Publications

Journal Articles

J. Lhermitte, C. R., S. S. Parker, J. M. Jackson and M. J. Monreal. Mg+2/0 as a reliable reference electrode for chloride melts. Submitted to *Journal of the Electrochemical Society*. (LA-UR-21-20290)

Reports

R. Andersson, A. D. Ab Initio Molecular Dynamics Simulations of Molten Actinide Chloride Salts. Unpublished report. (LA-UR-20-25841)

Presentation Slides

R. Andersson, A. D. and C. Jiang. Ab-Initio Molecular Dynamics Simulations of Actinide-Containing Molten Chloride Properties. Presented at *ORNL-GAIN MSR workshop*, Oak Ridge, Tennessee, United States, 2020-10-14 - 2020-10-14. (LA-UR-20-28172)

Jackson, J. M. Pyrochemical Processing of Actinides: Uranium and Plutonium Purification. Presented at *LANL Nuclear Forensics Workshop*, Los Alamos, New Mexico, United States, 2020-02-05 - 2020-02-07. (LA-UR-20-21332)

Jackson, J. M., M. J. Monreal, S. S. Parker, A. M. Long, S. C. Vogel and B. Winkler. Neutron Radiography for the Determination of Molten Chloride Viscosity, Density, and Homogeneity. Presented at *2019 AIChE*, Orlando, Florida, United States, 2019-11-10 - 2019-11-15. (LA-UR-19-31334)

Jackson, J. M. and M. J. Monreal. Preparation and Characterization of Molten Salt Systems. Presented at *TerraPower Site Visit*, Seattle, Washington, United States, 2019-08-19 - 2019-08-21. (LA-UR-19-28236)

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. and S. C. Vogel. Energy Resolved Neutron Imaging @ LANSCE: A Non-Destructive Tool for Interrogating Materials in Next Generation Nuclear Reactor Designs. Presented at *69th Annual Denver X-ray Conference*, Washington, District Of Columbia, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-24901)

Monreal, M. J. and J. M. Jackson. Measuring the Properties of Actinide-Molten Salts. . (LA-UR-20-24894)

Monreal, M. J. and J. M. Jackson. Molten Salt Thermophysical Property Measurements at Los Alamos National Laboratory. Presented at *Workshop for the Molten Salt Thermal Properties Working Group*, Columbia, South

Carolina, United States, 2020-07-14 - 2020-07-15. (LA-UR-20-25149)

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)

Posters

J. Lhermitte, C. R., M. J. Monreal, D. A. T. Rodriguez and J. M. Jackson. Electrochemical Investigation of Corrosion in Molten Salts. Presented at *Molten Salt Thermal Properties Working Group*, columbia, South Carolina, United States, 2020-03-17 - 2020-03-18. (LA-UR-20-22297)

The Dynamics of Systems Far From Equilibrium

Angel Garcia
20190496CR

Project Description

This project addresses the dynamics of fluid and metal systems out of equilibrium. The results are relevant for applications in carbon sequestration, ocean dynamics, and mixing of turbulent flows. At the most fundamental level, we will investigate computationally a range of fluid instabilities including low-Reynolds number porous media flows, multiphase compressible flows, and material interfaces in turbulent flows . Hydrodynamic instability, turbulence, and mixing have application in ocean and atmospheric modeling and in nuclear weapons physics.

Publications

Journal Articles

*Brady, E., S. Stevenson, D. Bailey, Z. Liu, D. Noone, J. Nusbaumer, B. L. Otto-Bliesner, C. Tabor, R. Tomas, T. Wong, J. Zhang and J. Zhu. The Connected Isotopic Water Cycle in the Community Earth System Model Version 1. 2019. *Journal of Advances in Modeling Earth Systems*. **11** (8): 2547-2566. (LA-UR-19-28472 DOI: 10.1029/2019MS001663)

Caravelli, F., F. C. Sheldon and F. L. Traversa. Global minimization via classical tunneling assisted by collective force field formation. Submitted to *Nature Physics*. (LA-UR-21-20810)

Caravelli, F., M. D. Saccone and C. Nisoli. On the Degeneracy of Spin Ice Graphs, and Its Estimate via the Bethe Permanent. Submitted to *Proceedings of the Royal Society A. Mathematical, Physical and Engineering Sciences*. (LA-UR-21-20434)

*Cheng, W., W. Weijer, W. M. Kim, G. Danabasoglu, S. G. Yeager, P. R. Gent, D. Zhang, J. C. H. Chiang and J. Zhang. Can the Salt-Advection Feedback Be Detected in Internal Variability of the Atlantic Meridional Overturning Circulation?. 2018. *Journal of Climate*. **31** (16): 6649-6667. (LA-UR-18-21355 DOI: 10.1175/JCLI-D-17-0825.1)

Ecke, R. E., O. Shishkina and X. Zhang. Boundary zonal flows in rapidly rotating turbulent thermal convection. Submitted to *Journal of Fluid Mechanics*. (LA-UR-20-27752)

*Gu, S., Z. Liu, A. Jahn, J. Rempfer, J. Zhang and F. Joos. Modeling Neodymium Isotopes in the Ocean Component of the Community Earth System Model (CESM1). 2019. *Journal of Advances in Modeling Earth Systems*. **11** (3): 624-640. (LA-UR-19-21453 DOI: 10.1029/2018MS001538)

*Gu, S., Z. Liu, J. Lynch-Stieglitz, A. Jahn, J. Zhang, K. Lindsay and L. Wu. Assessing the Ability of Zonal \xce\xb4 O Contrast in Benthic Foraminifera to Reconstruct Deglacial Evolution of Atlantic Meridional Overturning Circulation. 2019. *Paleoceanography and Paleoclimatology*. **34** (5): 800-812. (LA-UR-19-25176 DOI: 10.1029/2019PA003564)

*Hecht, M., M. Veneziani, W. Weijer, B. Kravitz, S. Burrows, D. Comeau, E. Hunke, N. Jeffery, J. Urrego-Blanco, W. Hailong, W. Shanlin, Z. Jiaxu, D. Bailey, C. Mills, P. Rasch and N. Urban. E3SMv0-HiLAT: A Modified Climate System Model Targeted for the Study of High-Latitude Processes. 2019. *Journal of Advances in Modeling Earth Systems*. **11** (8): 2814-2843. (LA-UR-18-27813 DOI: 10.1029/2018MS001524)

May, A., M. D. Saccone, A. M. Van Den Berg, J. Askey, M. Hunt and S. Ladak. Magnetic Charge Propagation upon a 3D Artificial Spin-ice. Submitted to *Nature Communications*. (LA-UR-21-22700)

Miller, J. M., T. M. Sprouse, C. L. Fryer, B. R. Ryan, J. C. Dolence, M. R. Mumpower and R. A. Surman. Full Transport General Relativistic Radiation Magnetohydrodynamics for Nucleosynthesis in Collapsars. Submitted to *Astrophysical Journal*. (LA-UR-19-30392)

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DeSantis, D. F., P. J. J. Wolfram and B. Alexandrov. Multiresolution Cluster Analysis - Addressing Trust in Climate Classification. Presented at *AMS Annual Meeting*, Boston, Massachusetts, United States, 2020-01-13 - 2020-01-17. (LA-UR-20-20382)

Jadrich, R. B. Accelerating materials design and ab initio simulation via statistical inference and machine learning. . (LA-UR-19-25374)

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Mathew, N. Multi-scale, multi-physics mechanics of engineering materials. . (LA-UR-19-22177)

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Mechanistic Studies of Human Disease

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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.

Publications

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Garcia, A. E., J. Janke, Y. Yu, V. Pomin, J. Zhao, C. Wang and R. Linhardt. Characterization of Heparin's Conformational Ensemble by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Spectroscopy. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-28381)

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Ke, R., S. Sanche, E. Romero-Severson and N. W. Hengartner. Estimating the reproductive number R0 of SARS-CoV-2 in the United States and eight European countries and implications for vaccination. 2021. *Journal of Theoretical Biology*. 110621. (LA-UR-20-25505 DOI: 10.1016/j.jtbi.2021.110621)

Mansbach, R. A., S. Chakraborty, T. K. Nguyen and S. Gnanakaran. Differential molecular signatures of the D and G forms the SARS-CoV2 trimeric Spike protein. Submitted to *Science Advances*. (LA-UR-20-25181)

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Shirin, A., Y. T. Lin and F. Sorrentino. Data-driven Optimized Control of the COVID-19 Epidemics. Submitted to *Nature Communications*. (LA-UR-20-26630)

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Migliori, A. D. Slides for FNLCR collaborators. . (LA-UR-19-32620)

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Rosenberger, D. G. Using Kirkwood-Buff Integrals to estimate diffusion in mixtures.. . (LA-UR-20-28325)

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Information Science and Technology

Enabling Predictive Scale-Bridging Simulations through Active Learning

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Project Description

Exascale supercomputers that will arrive in the next few years offer tremendous computational power, if one can coordinate the approximately one billion different calculations that are occurring at any given time. Our project combines these exciting advances in computing architectures with similarly exciting advances in machine learning algorithms to enable computational science and engineering simulations with greater physical fidelity, combining molecular-scale simulations with continuum fluid dynamics ones. Just as understanding nanomaterial properties has been a grand challenge over the past two decades, understanding fluids in complex nanopores is the next frontier. Our computational framework for incorporating nanoscale physics will enable efficient extraction of subsurface energy (hydrocarbon and geothermal) from tight unconventional resources which have proved to be extremely challenging. Similarly, we expect to be able to efficiently and accurately account for complex atomistic effects such as non-local transport in inertial confinement fusion (ICF) simulations, providing a valuable computational tool for understanding whether ignition is ultimately achievable and, if yes, suggest practical avenues for controlling mix, instabilities, and heat loss from the hot spot. Our active learning approach will bring about transformational advances in the way nanoconfinement effects of fluids are modeled in these and other applications.

Publications

Journal Articles

*Bakhshian, S., M. Murakami, S. A. Hosseini and Q. Kang. Scaling of Imbibition Front Dynamics in Heterogeneous Porous Media. 2020. *Geophysical Research Letters*. **47** (14): e2020GL087914. (LA-UR-20-22139 DOI: 10.1029/2020GL087914)

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Gong, Y., M. Z. S. Mehana, I. El-monier and H. S. Viswanathan. Proppant Placement in Complex Fracture Geometries: A Computational Fluid Dynamics. Submitted to *Scientific Reports*. (LA-UR-19-29884)

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Li, Y. W., M. Lupo Pasini, J. Yin, J. Zhang, K. M. Barros and M. Eisenbach. Fast and stable deep-learning predictions of material properties of solid solution alloys. Submitted to *Journal of Physics: Condensed Matter*. (LA-UR-20-27481)

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Wang, K., Y. Chen, M. Z. S. Mehana, N. E. Lubbers, K. Bennett, Q. Kang, H. S. Viswanathan and T. C. Germann. A physics-informed and hierarchically regularized data-driven model for predicting fluid flow through porous media. Submitted to *Journal of Computational Physics*. (LA-UR-20-27444)

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Chen, Y. Recent progresses in image-based pore-scale multiphase flow simulations using advanced models and GPU acceleration. Presented at *Los Alamos - Arizona Days*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-19. (LA-UR-20-23629)

Haack, J. R. Towards Enabling Predictive Scale-Bridging Simulations through Active Learning. . (LA-UR-20-23366)

Haack, J. R. Scale Bridging through Active Learning. . (LA-UR-21-20131)

Junghans, C. Novel Approaches to Multi-Scale Modeling. . (LA-UR-21-22275)

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Pachalieva, A. A. Learning Lattice Boltzmann Methods via H-functions. Presented at *CNLS Postdoc Seminar*, Los Alamos, New Mexico, United States, 2020-10-01 - 2020-10-01. (LA-UR-20-27736)

Pachalieva, A. A. and A. Wagner. Deriving LBM collision operator using the Coarse-Graining MDLG Approach. Presented at *29th International Conference on Discrete Simulation of Fluid Dynamics (DSFD 2020)*, Viterbo, Italy, 2020-07-13 - 2020-07-17. (LA-UR-20-25144)

Pavel, R. S., C. Junghans and T. C. Germann. Workflow Requirements for Active Learning Enabled Scale-Bridging Simulations. . (LA-UR-21-20939)

Rosenberger, D. G. Learning diffusion coefficients of particles with the help of thermodynamics. Presented at *2019 ALCF Simulation, Data, and Learning Workshop*, Argonne, Illinois, United States, 2019-10-01 - 2019-10-03. (LA-UR-19-29611)

Rosenberger, D. G. Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21573)

Rosenberger, D. G. Using machine learning to estimate ideal/non ideal mixing in binary ionic mixtures.. . (LA-UR-21-21248)

Rosenberger, D. G., N. E. Lubbers and T. C. Germann. Evaluating diffusion and the thermodynamic factor for binary ionic mixtures.. Presented at *Frontiers in Machine Learning for the Physical Sciences*, Virtual event, California, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28065)

Viswanathan, H. S. Flow and Fracture in Microstructure Accelerated by Machine Learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-20 - 2019-02-20. (LA-UR-19-21272)

Posters

S. Mehana, M. Z., Q. Kang and H. S. Viswanathan. On the Molecular Modeling of Hydrocarbon Behavior in Shale Nano-pores. Presented at *LANL postdoc Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28695)

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Sagert, I., J. R. Haack, A. Diaw, C. Junghans, B. Keenan, N. E. Lubbers, M. McKerns, R. S. Pavel and D. Livescu. A 3D Multi-Species Kinetic-Fluid Coupling Technique for HEDP Simulations. Presented at *International Conference on Numerical Simulations of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28767)

Other

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. Simulation data of fluid displacement in sandstone near entire-core scale. Dataset. (LA-UR-21-22272)

Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics

Boian Alexandrov
20190020DR

Project Description

The world's data is the most valuable exponentially-growing resource. Terabyte scale datasets are generated every minute by massive computer simulations, large-scale experiments, and global surveillance systems. Analyses of these data are of crucial importance for global security and directly related to Department of Energy mission-critical research areas. Development of machine learning (ML) techniques for efficient and robust data analyses is of paramount importance to perform timely, accurate, and meaningful data interpretation. Our project addresses this need by developing a novel ML methodology and a unique high-performance computing toolbox to perform data analyses and extract meaningful and interpretable features from high-dimensional extra-large datasets. High-dimensional data are naturally organized in tensors (multi-dimensional arrays) and our methodology will focus on cutting-edge tensor-based ML methods utilizing novel techniques. We will target terabyte and petabyte scale datasets in this project but if this high-risk/high-reward research is successful, the developed high-performance computing tools will be able to address larger problems. The new methodology will be important for DOE, the National Nuclear Security Administration, National Security Agency, Nuclear Regulatory Commission, Enviornmental Protection Agency, National Institutes of Health, and other agencies, placing the Laboratory in a leadership position in the field of Big-Data Analytics.

Publications

Journal Articles

Ahmmed, B., M. K. Mudunuru, S. Karra, S. C. James and V. V. Vesselinov. A comparative study of machine learning models for predicting the state of reactive mixing. 2021. *Journal of Computational Physics*. 110147. (LA-UR-20-21737 DOI: 10.1016/j.jcp.2021.110147)

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Ahmmed, B., S. Karra, V. V. Vesselinov and M. K. Mudunuru. Machine Learning to Discover Mineral Trapping Signatures due to CO2 Injection. Submitted to *International Journal of Greenhouse Gas Control*. (LA-UR-21-20069)

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Alexandrov, B., B. Zhu, M. L. Poeta, M. Costantini, T. Zhang, J. Shi, S. S. Sentinelli, V. Pompeo, M. Cardelli, B. Otlu, X. Hua, K. Jones, S. Brodie, J. R. Toro, M. Yeager, M. Wang, B. Hicks, L. B. Alexandrov, K. M. Brown, S. Chanock, V. M. Fazio, M. Gallucci and M. T. Landi. Intratumor heterogeneity and clonal expansion cascade in papillary renal cell carcinoma. Submitted to *Genome Biology*. (LA-UR-18-31218)

Alexandrov, B., C. A. Lopez Bautista and S. Gnanakaran. Unsupervised Machine Learning for Analysis of Coexisting Lipid Phases and Domain Growth in Biological Membranes. Submitted to *JCTC*. (LA-UR-18-29079)

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonic Polyadic Decomposition with Rank Deficient Factors. Submitted to *SIAM Journal on Mathematics of Data Science*. (LA-UR-19-29298)

Alexandrov, B., K. O. Rasmussen, G. Weissman, G. Bel, U. Yermiyahu, A. Ben-Gal and O. Dahan. Effects of salinity and soil heterogeneity on water, nitrate and bromide flow under agricultural fields. Submitted to *Vadose Zone Journal*. (LA-UR-19-31560)

Alexandrov, B., M. Karimi, V. Petkova, J. M. Asara, M. Griffin and A. Usheva. Aberrant cardiac energy metabolism in metabolic syndrome: insight from metabolomics and a pig model. Submitted to *Scientific Reports*. (LA-UR-19-25878)

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*Carrillo-Cabada, H., E. Skau, G. Chennupati, B. Alexandrov and H. Djidjev. An Out of Memory tSVD for Big-Data Factorization. *IEEE Access*. **8**: 107749-107759. (LA-UR-20-22236 DOI: 10.1109/ACCESS.2020.3000508)

*Chennupati, G., R. Vangara, E. Skau, H. Djidjev and B. Alexandrov. Distributed non-negative matrix factorization with determination of the number of latent features. 2020. *The Journal of Supercomputing*. **76** (9): 7458-7488. (LA-UR-20-20469 DOI: 10.1007/s11227-020-03181-6)

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Karra, S., B. Ahmmed and M. K. Mudunuru. Dataset for Machine Learning Analysis of Reactive Mixing under Anisotropy and Heterogeneity. Submitted to *Data in brief, Elsvier*. (LA-UR-21-20064)

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O'Malley, D., H. N. Djidjev and B. Alexandrov. Boolean Tensor Factorization with QuantumAnnealers. Submitted to *npj Quantum Information*. (LA-UR-20-21860)

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R. Pelofske, E. A., G. Hahn, D. O'Malley, H. N. Djidjev and B. Alexandrov. Boolean Hierarchical Tucker Networks on Quantum Annealers. Submitted to *Large-Scale Scientific Computations*. (LA-UR-21-22363)

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Prakash, D. J., L. Denoyer, R. Vangara, J. M. Baca, F. van Swol and D. N. Petsev. Ionic Size Effects on the Properties of Charge Regulating Electric Double Layers. Submitted to *Physical Review E*. (LA-UR-21-20082)

Truong, D. P., E. W. Skau, V. I. Valtchinov and B. Alexandrov. Determination of Latent Dimensionality in International Trade Flow. Submitted to *Machine Learning: Science and Technology*. (LA-UR-20-21947)

*Vangara, R., K. O. Rasmussen, D. N. Petsev, G. Bel and B. S. Alexandrov. Identification of anomalous diffusion sources by unsupervised learning. 2020. *Physical Review Research*. **2** (2): 023248. (LA-UR-20-23646 DOI: 10.1103/PhysRevResearch.2.023248)

Conference Papers

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Bhattarai, M., G. Chennupati, E. W. Skau, R. Vangara, H. N. Djidjev and B. Alexandrov. Distributed Non-negative Tensor Train Factorization. Presented at *IEEE High-Performance Extreme Computing Conference (HPEC '20)*. (Boston, Massachusetts, United States, 2020-09-22 - 2020-09-24). (LA-UR-20-24426)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics*. (Online, New Mexico, United States, 2020-11-09 - 2020-11-10). (LA-UR-20-26304)

Nasrin, A., R. Vangara, G. Chennupati, B. Alexandrov, H. N. Djidjev and S. Amarda. Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures. Presented at *IEEE International Conference on Bioinformatics and Biomedicine*. (San Diego, California, United States, 2019-11-18 - 2019-11-21). (LA-UR-19-30412)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Optimizing the spin reversal transform on the D-Wave 2000Q. Presented at *ICRC 2019*. (San Mateo, California, United States, 2019-11-06 - 2019-11-08). (LA-UR-19-25307)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Peering into the Anneal Process of a Quantum Annealer. Presented at *PDCAT 2019*. (Gold Coast, Australia, 2019-12-05 - 2019-12-07). (LA-UR-19-27870)

Pulido, J. J., J. M. Patchett, M. Bhattarai, B. Alexandrov and J. P. Ahrens. Selection of Optimal Salient Time Steps by Non-negative Tucker Tensor Decomposition. Presented at *EuroVis 2021 - Conference on Visualization*. (Zurich, Switzerland, 2021-06-14 - 2021-06-18). (LA-UR-21-22070)

Sanchez, G., E. W. Skau and B. Alexandrov. QUATERNION NON-NEGATIVE MATRIX FACTORIZATION WITH MODEL SELECTION FOR SPECTROPOLARIMETRIC IMAGING. Presented at *2021 IEEE International Conference on Acoustics, Speech and Signal Processing*. (Toronto, Canada, 2021-06-06 - 2021-06-11). (LA-UR-20-28403)

Vangara, R., E. W. Skau, G. Chennupati, H. N. Djidjev, M. Bhattarai, T. E. I. Tierney, J. P. Smith, V. Stanev and B. Alexandrov. Finding the Number of Topics with Semantic Nonnegative Matrix Factorization. Presented at *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML PKDD) 2020*. (Ghent, Belgium, 2020-09-14 - 2020-09-18). (LA-UR-20-22845)

Vangara, R., E. W. Skau, G. Chennupati, H. N. Djidjev, T. E. I. Tierney, J. P. Smith, M. Bhattarai, V. Stanev and B. Alexandrov. Semantic Nonnegative Matrix Factorization with Automatic Model Determination for Topic Modeling. Presented at *19th IEEE International Conference On Machine Learning And Applications*. (MIAMI, Florida, United States, 2020-12-14 - 2020-12-17). (LA-UR-20-28028)

Reports

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. distNMFk: Distributed Non-negative Matrix Factorization to Extract Optimal Number of Features. Unpublished report. (LA-UR-19-25810)

DeSantis, D. F., L. Van Roekel, B. Alexandrov and R. Vangara. Hidden Climate Signatures and Mechanisms in Energy Exascale Earth System Model Data. Unpublished report. (LA-UR-21-21294)

Presentation Slides

Ahmmed, B. Numerical Modeling, Uncertainty Analyses, and Machine Learning for Decision Support in the Geosciences. . (LA-UR-20-23178)

Ahmmed, B. Supervised and Unsupervised Machine Learning to Understanding Reactive-transport Data. . (LA-UR-20-23812)

Ahmmed, B., N. Lautze, V. V. Vesselinov, D. Dores and M. K. Mudunuru. Unsupervised Machine Learning to Extract Dominant Geothermal Attributes\xc2\xa0 in Hawaii Island Play Fairway Data. Presented at *Geothermal Resources Council*, Reno, Nevada, United States, 2020-10-18 - 2020-10-23. (LA-UR-20-26170)

Ahmmed, B., V. V. Vesselinov and M. K. Mudunuru. Non-negative Matrix Factorization to Discover Dominant Attributes in Utah FORGE Data. Presented at *Geothermal Resources Conference*, Reno, Nevada, United States, 2020-10-18 - 2020-10-23. (LA-UR-20-26171)

Ahmmed, B., V. V. Vesselinov and M. K. Mudunuru. Machine Learning to Characterize Regional Geothermal Reservoirs in the Western USA. Presented at *GSA*, Online, Colorado, United States, 2020-10-26 - 2020-10-30. (LA-UR-20-27654)

Alexandrov, B. Unsupervised Phase Mapping of X-ray Diffraction Data by Nonnegative Matrix Factorization. Presented at *Invited talk in UC Irvine University on AI and Materials*, Irvine, California, United States, 2019-11-21 - 2019-11-21. (LA-UR-19-31561)

Alexandrov, B. Nonnegative Tensor Nets and Extraction of Latent Variables Targeting Discovery. . (LA-UR-20-25418)

Alexandrov, B. and T. Mina. Test with Gaussian signals. . (LA-UR-20-24155)

Bhattarai, M., G. Chennupati, E. W. Skau, R. Vangara, H. N. Djidjev and B. Alexandrov. Distributed Non-Negative Tensor Train Decomposition. Presented at *IEEE High Performance Extreme Computing Conference (HPEC '20)*, Boston, Massachusetts, United States, 2020-09-21 - 2020-09-25. (LA-UR-20-27354)

Chennupati, G. Massively Parallel Big-Data Nonnegative Factorization. Presented at *Internal DR appraisal review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21162)

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. Distributed Non-negative Matrix Factorization with Model Determination. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Los Alamos, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29294)

Eren, M. E., J. S. Moore and B. Alexandrov. Anomalous Event Detection using Non-Negative Poisson Tensor Factorization. . (LA-UR-20-25933)

Eren, M. E., J. S. Moore and B. Alexandrov. Anomalous Event Detection using Non-Negative Poisson Tensor Factorization. . (LA-UR-20-26093)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics (ISI)*, Online, New Mexico, United States, 2020-11-09 - 2020-11-10. (LA-UR-20-28568)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-10. (LA-UR-20-28561)

Kober, E. M., M. F. Francis, R. Vangara and B. Alexandrov. Tensor Factorization Applied to the Reaction Analysis of Energetic

Materials. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29243)

Marcillo, O. E. and J. K. MacCarthy. Mapping Tonal Noise in the Continental US. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29507)

Nebgen, B. T., J. K. MacCarthy and B. Alexandrov. Non-Negative Tensor Factorization for Interpretable Unsupervised Signal Discovery in Continuous Seismic Data. Presented at *Seismological Society of America National Meeting*, Seattle, Washington, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23443)

Nebgen, B. T., R. Vangara, S. Kuksova, M. A. Hombrados Herrera and B. Alexandrov. Machine Learning for Automated Feature Recognition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29238)

O'Malley, D. Tensor factorization with quantum annealing. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29405)

Skau, E. W. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29328)

Vangara, R., B. T. Nadiga and B. Alexandrov. Tensor Methods for analyzing Sea Ice Thickness in Arctic.. Presented at *AI4ESP*, Los Alamos, New Mexico, United States, 2021-01-08 - 2021-01-08. (LA-UR-21-20130)

Vesselinov, V. V. Physics-Informed Machine Learning Methods for Data Analytics and Model Diagnostics. Presented at *M3 DRIVE Science Center:*, Los Alamos, New Mexico, United States, 2019-05-14 - 2019-05-14. (LA-UR-19-24562)

Vesselinov, V. V., B. Ahmmed and M. K. Mudunuru. Unsupervised Machine Learning to discover attributes that characterize low, moderate, and high-temperature geothermal resources. Presented at *Geothermal Resources Conference*, Reno, Nevada, United States, 2020-10-18 - 2020-10-23. (LA-UR-20-26184)

Posters

Bhattarai, M., R. Vangara, G. Chennupati, J. M. Patchett, J. P. Ahrens and B. Alexandrov. pyDnMFk: A Python implementation of Distributed Non-Negative Matrix Factorization with determination of Rank. Presented at *LDRD Project Review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21243)

Carrillo Cabada, H. A., E. W. Skau, G. Chennupati, H. N. Djidjev and B. Alexandrov. Out-of-Core Singular Value Decomposition for the Tensor Train Decomposition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29330)

Carrillo, H., E. W. Skau, G. Chennupati, H. N. Djidjev and B. Alexandrov. Out-of-Core Singular Value Decomposition for the Tensor Train Decomposition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29862)

Francis, M. F., E. M. Kober, B. Alexandrov, R. Vangara and B. T. Nebgen. Machine Learning of Transient Chemical Kinetics: NMF, NN, and SVR of HMX. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29274)

Hombrados Herrera, M. A., R. Vangara, E. W. Skau and B. Alexandrov. Methods for determination of dimensionality of latent features: Principal Angles and PCAk. Presented at *AI and Tensor Factorizations for Physical, Chemical and Biological Systems.*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-19. (LA-UR-19-29467)

Kuksova, S., B. Alexandrov and K. O. Rasmussen. Nonegative Tensor Train Analysis for Feature Extraction. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29464)

M. Mallory, E. J., B. T. Nebgen, O. E. Marcillo, J. K. MacCarthy, K. O. Rasmussen and B. Alexandrov. Tensor Decomposition for Mars Seismology. Presented at *Elizabeth Mallory*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29281)

M. Mallory, E. J., T. B. Peery and M. F. Francis. Statistical Representations and Unbiased Metrics for Stable Isotope Fractionation. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32132)

Nasrin, A., R. Vangara, G. Chennupati, B. Alexandrov, H. N. Djidjev and S. Amarda. Non-Negative Matrix Factorization for Decoy Selection from Ensembles. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Los Alamos, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29332)

Rasmussen, K. O., E. J. M. Mallory, B. T. Nebgen, O. E. Marcillo, J. K. MacCarthy and B. Alexandrov. Tensor Decomposition for Mars Seismology. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, SANTA FE, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29777)

Rasmussen, K. O., G. Bel, R. Vangara, D. Petsev and B. Alexandrov. Unsupervised Learning for Anomalous Diffusion Source Identification. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological*

Systems, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29256)

Rasmussen, K. O., S. Kuksova and B. Alexandrov. Nonnegative Tensor Train Analysis for Feature Extraction. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29776)

Rijal, B., B. T. Nebgen, C. A. Neale and B. Alexandrov. Tensor Factorization for Protein Conformation Identification. Presented at *AI and Tensor Factorization for Physical, Chemical and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29311)

Skau, E. W. Symmetric Tucker Rank Determination. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29329)

Truong, D., E. W. Skau and B. Alexandrov. Symmetric Tucker Rank Determination. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29863)

Vangara, R., E. M. Kober and B. Alexandrov. Tensor Methods for Reaction Analysis of Energetic Materials and High Explosives. Presented at *DR Midterm Review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21230)

Vangara, R., G. Chennupati and B. Alexandrov. Symmetric Non-Negative Matrix Factorization with PAC for Estimating Number of Clusters. Presented at *Conference on Data Analysis (CODA 2020)*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21809)

Machine Learning for Turbulence

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20190059DR

Project Description

Machine Learning for Turbulence will develop a novel framework which will dramatically improve models used in hydrodynamic codes at Los Alamos National Laboratory and other National Laboratories of the Department of Energy. The models are significant for such mission critical applications as weapons design and simulations, modeling and predictive weather and understanding astrophysical phenomena. Our main hypothesis is that an automatic design of the hydrodynamic closures is achievable through new approach, coined Physics Informed Machine Learning, suggesting and developing smart embedding of the underlying physics into Machine Learning techniques. We will test the hypothesis by developing a theoretical and algorithmic methods guided by insight from the hydrodynamic applications of interest. We will examine the power of the new tools in bridging existing approaches. Thus, application agnostic machine learning will be augmented with the physical constraints reflecting basic hydrodynamic symmetries. Complementary, current Laboratory closure models of turbulence will be enhanced by embedding into them Neural Networks thus allowing automatic evaluation, larger time steps and faster in line computations.

Publications

Journal Articles

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Taming Defects in Quantum Computers

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Project Description

Since the enactment of the Comprehensive Nuclear Test Ban Treaty, stockpile stewardship has relied heavily on computer simulations of weapons effects. Until recently, continuous improvements in supercomputing technology have made it possible to increase the physics fidelity of these simulations without unduly slowing them down. Alas, with all of the low-hanging fruit long since picked, performance improvements are becoming increasing elusive with each new generation of supercomputers. The situation existentially threatens the National Nuclear Security Administration's ability to ensure the safety, security, and effectiveness of America's nuclear stockpile. Quantum computing is a new technology that offers the potential of drastically improved computational speed—well beyond what any supercomputer in the foreseeable future is capable of. Unfortunately, early quantum computers are extremely unreliable and extremely difficult to program. Our project will address both those issues. We will develop a framework that enables NNSA computational scientists to describe a mapping of inputs to outputs and automatically converts that mapping into a quantum algorithm, and one that is customized to work around a particular quantum computer's individual shortcomings. This will enable stockpile stewardship simulations to continue their prior trajectory of ever-improving accuracy and ever-improving utility to national security.

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Quantum Chemistry using Quantum Computers

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Project Description

Quantum computers (QC) promise to be a game changer for materials science modeling, an appropriate implementation and 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.

Publications

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Mniszewski, S. M. Quantum Chemistry In Pieces. . (LA-UR-20-23201)

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Prioritizing the Prior: Advanced Inversion Algorithms for Scientific Data Analysis

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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.

Publications

Journal Articles

Bacak, M., J. Valsecchi, J. Capek, E. Polatidis, A. Kaestner, A. Arabi-Hashemi, I. I. Kruk, C. Leinenbach, A. M. Long, A. S. Tremsin, S. C. Vogel, E. B. Watkins and M. Strobl. Neutron dark-field imaging applied to porosity and deformation-induced phase transitions in additively manufactured steels. Submitted to *Materials & Design*. (LA-UR-20-25975)

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Goyes-Penafiel, P., E. Vargas, C. V. Correa, W. Agudelo, B. E. Wohlberg and H. Arguello. A Consensus Equilibrium Approach for 3D Land Seismic Shots Recovery. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-21-22053)

Hovey, L. D. and M. L. Klasky. Parametric Generation of 1D Sedov Point Explosions in Varying Ambient Media using Dynamic Mode Decomposition. Submitted to *Shock Waves*. (LA-UR-21-21016)

Lehmann, E. H., D. Mannes, M. Strobl, B. Walfort, A. Losko, B. Schillinger, M. Schulz, S. C. Vogel, D. Schaper, D. C. Gautier and D. A. Newmark. Improvement in the spatial resolution for imaging with fast neutrons. 2020. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. 164809. (LA-UR-20-26818 DOI: 10.1016/j.nima.2020.164809)

Lin, Y. Data-Driven Seismic Waveform Inversion: A Study on the Robustness and Generalization. 2020. *IEEE Transactions on Geoscience and Remote Sensing*. **58** (10): 6900-6913. (LA-UR-19-24398 DOI: 10.1109/TGRS.2020.2977635)

Lin, Y., J. P. Theiler and B. E. Wohlberg. Physics-Consistent Data-driven Waveform Inversion with Adaptive Data Augmentation. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-20-22488)

Lin, Y., Q. Zeng, S. Feng and B. E. Wohlberg. InversionNet3D:High-Resolution 3D Full Waveform Inversion with Efficient Encoder-Decoder Network. Submitted to *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*. (LA-UR-21-22293)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Connecting the Dots: InSitu 4D Seismic Monitoring of CO2 Storage with Spatio-temporal CNN. Submitted to *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*. (LA-UR-21-22295)

Lin, Y., S. Feng and B. E. Wohlberg. Multi-scale Data-driven Computational Seismic Imaging: A Field Data Study. Submitted to *Nature Machine Intelligence*. (LA-UR-21-20004)

Losko, A. S., L. L. Daemen, P. Hosemann, H. Nakotte, A. S. Tremsin, S. C. Vogel, P. Wang and F. Wittmann. Separation of Uptake of Water and Ions in Porous Materials using Energy Resolved Neutron Imaging. Submitted to *JOM*. (LA-UR-19-32650)

Losko, A. S. and S. C. Vogel. 3D Isotope Density Measurements by Energy-Resolved Neutron Imaging. Submitted to *Nature*. (LA-UR-19-32651)

Lu, J., Y. Sun, W. Gan, X. Xu, B. E. Wohlberg and U. Kamilov. SGD-Net: Efficient Model-Based Deep Learning with Theoretical Guarantees. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-21-20696)

McKeown, M., S. Brusatte, T. Williamson, J. Schwab, T. Carr, I. Butler, A. Muir, K. Schroeder, M. A. Espy, J. F. Hunter, A. S. Losko, R. O. Nelson, D. C. Gautier and S. C. Vogel. Neurosensory and sinus evolution as tyrannosauroid dinosaurs developed giant size: insight from the endocranial anatomy of Bistahieversor sealeyi. Submitted to *The Anatomical Record*. (LA-UR-19-32710)

Sun, Y., J. Liu, M. Xie, B. E. Wohlberg and U. S. Kamilov. CoIL: Coordinate-based Internal Learning for Imaging Inverse Problems. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-21-21526)

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Xie, M., Y. Sun, J. Liu, B. E. Wohlberg and U. S. Kamilov. Joint Reconstruction and Calibration Using Regularization by Denoising. Submitted to *IEEE Signal Processing Letters*. (LA-UR-20-29788)

Xu, X., J. Liu, Y. Sun, B. E. Wohlberg and U. Kamilov. Boosting the Performance of Plug-and-Play Priors via Denoiser Scaling. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-19-32413)

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Klasky, M. L., L. A. Pfister, J. L. S. Disterhaupt, M. T. McCann and S. Ravishankar. Descattering and Reconstruction in MultiMaterial Polyenergetic X-Ray Tomography Using Local Scatter Models. Presented at *OSA Digital Holography and Three-Dimensional Imaging Topical Meeting (DH)*. (Vancover, Canada, 2021-07-19 - 2021-07-19). (LA-UR-21-22245)

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Lin, Y., J. D. Moulton, B. E. Wohlberg, E. Cromwell and X. Chen. CycleFCN: A Physics-Informed Data-driven SeismicWaveform Inversion. Presented at *Society of Exploration Geophysics Annual Meeting*. (houston, Texas, United States, 2020-10-11 - 2020-10-11). (LA-UR-20-22907)

Lin, Y. and B. E. Wohlberg. Physically Realistic Training Data Building for Data-driven Full-waveform Inversion and Traveltime Tomography. Presented at *Society of Exploration Geophysics Annual Meeting*. (houston, Texas, United States, 2020-10-11 - 2020-10-11). (LA-UR-20-22908)

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)

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Sun, Y., J. Liu, Y. Sun, B. E. Wohlberg and U. S. Kamilov. Async-RED: A Provably Convergent Asynchronous Block Parallel Stochastic Method using Deep Denoising Priors. Presented at *International Conference on Learning Representations*. (Vienna, Austria, 2021-05-04 - 2021-05-04). (LA-UR-20-28190)

Reports

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Klasky, M. L., B. T. Nadiga, J. L. S. Disterhaupt, T. Wilcox, L. D. Hovey, T. Mockler, C. L. Fryer, E. N. Loomis, A. L. Hungerford, S. K. Sjue, L. A. Pfister and Y. Han. UNCERTAINTIES IN DENSITY AND SIMULATION PARAMETERS FOR RADIOGRAPHIC RECONSTRUCTIONS USING MACHINE LEARNING. Unpublished report. (LA-UR-20-24065)

Vogel, S. C., T. Balke, C. A. Bouman, L. Capriotti, J. M. Harp, A. M. Long, D. Schaper, A. S. Tremsin and B. E. Wohlberg. First Examination of Irradiated Fuel with Pulsed Neutrons at LANSCE – Preliminary Results. Unpublished report. (LA-UR-20-27504)

Vogel, S. C. and E. B. Watkins. Neutron Imaging Using Grating Interferometry: Exploiting phase contrast and dark-field imaging for <1\xce\xbcm feature detection in bulk materials. Unpublished report. (LA-UR-20-27576)

Presentation Slides

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Garcia Cardona, C. Advanced Inversion Algorithms for Scientific Data Analysis. . (LA-UR-21-21830)

Garcia Cardona, C., B. E. Wohlberg and Y. Sun. Learning Convolutional Sparse Representations. Presented at *Join Mathematics Meetings*, Denver, Colorado, United States, 2020-01-15 - 2020-01-18. (LA-UR-20-20492)

Garcia Cardona, C., R. Kannan, T. Johnston, T. Proffen and S. K. Seal. Structure Prediction from Neutron Scattering Profiles: A Data Sciences Approach. Presented at *IEEE BigData 2020*, Virtual Conference, New Mexico, United States, 2020-12-10 - 2020-12-13. (LA-UR-20-29777)

Klasky, M. L., C. Bouman, J. L. S. Disterhaupt, M. A. Espy, J. Fessler, M. Hossein, E. Guardincerri, L. D. Hovey, O. Korobkin, A. Lahiri, M. McCann, B. T. Nadiga, B. M. Patterson, L. A. Pfister, S. K. Sjue, S. Ravishankar, D. L. Sanzo, T. Wilcox and B. E. Wohlberg. EREBUS Coupled Hydrodynamic Radiographic Dynamic Reconstruction & Limited View Reconstructions. . (LA-UR-21-22694)

Klasky, M. L., C. Bouman, J. L. S. Disterhaupt, O. Korobkin, M. Hossein, L. D. Hovey, M. McCann, B. T. Nadiga, L. A. Pfister, S. Ravishankar, T. Wilcox, B. E. Wohlberg and D. L. Sanzo. Physics Informed Dynamic Radiography. Presented at *LDRD FY Review*, Los Alamos, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30149)

Klasky, M. L., T. Wilcox, J. L. S. Disterhaupt, Y. Han, L. A. Pfister, S. Ravishankar and M. McCann. Towards a unified radiographic/hydrodynamic approach to obtaining accurate density from dynamic radiographic measurements. Presented at *Dynamic Radiography Introduction*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-18. (LA-UR-20-23590)

Klasky, M. L., Y. Z. Watkins, E. W. Skau, K. A. Stults and L. Hung. MAD using INRAD and Radiography. . (LA-UR-20-21612)

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Lin, Y., S. Feng and B. E. Wohlberg. Physically Realistic Training Data Construction for Data-driven Full-waveform Inversion and Traveltime Tomography. Presented at *Society of Exploration Geophysics Annual Meeting*, Houston, Texas, United States, 2020-10-11 - 2020-10-11. (LA-UR-20-26781)

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)

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)

Vogel, S. C., A. M. Long, D. C. Gautier, J. Valloton and H. Henein. Neutron and X-ray Characterization of D2 Tool Steel Solidified in Microgravity. Presented at *Center for Space and Earth Science Microgravity Symposium*, los alamos, New Mexico, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28477)

Vogel, S. C., J. R. Angell, T. Balke, D. T. Carver, L. Capriotti, A. E. Craft, J. Harp, P. Hosemann, J. Lin, A. M. Long, E. J. Larson, K. J. Mcclellan and D. Schaper. Characterization of Irradiated Nuclear Fuels with Pulsed Neutrons. Presented at *TMS Annual Meeting*, virtual, New Mexico, United States, 2021-03-14 - 2021-03-14. (LA-UR-21-22081)

Wohlberg, B. E., C. Garcia Cardona, S. C. Vogel, T. Balke, A. M. Long, M. L. Klasky, K. M. Mertes, J. L. Barber, Y. Lin, L. A. Pfister, S. Feng, O. Korobkin and J. F. Hunter. LDRD Project 20200061DR Review. . (LA-UR-20-30159)

In-Situ Inference: Bringing Advanced Data Science into Exascale Simulations

Earl Lawrence
20200065DR

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.

Publications

Journal Articles

Biswas, A., S. Dutta, E. C. Lawrence, J. M. Patchett, J. C. Calhoun and J. P. Ahrens. Probabilistic Data-Driven Sampling via Multi-Criteria Importance Analysis. Submitted to *IEEE Transactions on Visualization and Computer Graphics*. (LA-UR-20-20029)

Katzfuss, M., J. Guinness and E. C. Lawrence. Scaled Vecchia approximation for fast computer-model emulation. Submitted to *Technometrics*. (LA-UR-20-23222)

W. Myren, S. T. and E. C. Lawrence. Comparison of Emulation Techniques for Bayesian Calibration. Submitted to *Statistical Analysis and Data Mining*. (LA-UR-20-25141)

Conference Papers

Hazarika, S., A. Biswas, E. C. Lawrence and P. J. J. Wolfram. Probabilistic Principal Component Analysis Guided Spatial Partitioning of Multivariate Ocean Biogeochemistry Data. Presented at *Visualization in Environmental Sciences 2021 (EnvirVis 2021)*. (Zurich, Switzerland, 2021-06-14 - 2021-06-14). (LA-UR-21-22299)

Hazarika, S., A. Biswas, P. J. J. Wolfram, E. C. Lawrence and N. M. Urban. Relationship-aware Multivariate Sampling Strategy for Scientific Simulation Data. Presented at *IEEE Visualization Conference 2020*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-20-24913)

Reports

Lawrence, E. C., A. Biswas, L. Van Roekel and N. Urban. In Situ Inference for Earth System Predictability. Unpublished report. (LA-UR-21-21483)

Urban, N. M., E. C. Lawrence and A. Biswas. In-Situ Inference: Bringing Advanced Data Science Into Exascale Simulations. Unpublished report. (LA-UR-20-20586)

Presentation Slides

Biswas, A. In Situ Data Reduction and Statistical Inference. . (LA-UR-20-30474)

Grosskopf, M. J. In Situ Inference for Exascale Scientific Computing. Presented at *Joint Statistical Meeting*, Online, New Mexico, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-25961)

Hazarika, S., A. Biswas, P. J. J. Wolfram, E. C. Lawrence and N. M. Urban. Relationship-aware Multivariate Sampling Strategy for Scientific Simulation Data. Presented at *IEEE Visualization 2020*, Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25. (LA-UR-20-27080)

Hazarika, S., A. Biswas, P. J. J. Wolfram, E. C. Lawrence and N. M. Urban. Relationship-aware Multivariate Sampling Strategy for Scientific Simulation Data. Presented at *IEEE Visualization 2020*, Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25. (LA-UR-20-27078)

Jordanova, V. K. Key Aspects of Self-Consistent Ring Current Modeling. . (LA-UR-20-25791)

Jordanova, V. K. Inner Magnetosphere Plasma and Field Dynamics. Presented at *PWING-ERG Online Conference and School*, Nagoya, Japan, 2021-03-08 - 2021-03-12. (LA-UR-21-20090)

Lawrence, E. C. Computer Experiments at Los Alamos National Laboratory: Life on Mars and Really Big Computers. Presented at *The University of Michigan Department of Statistics Distinguished Alumni Speaker Series*, Ann Arbor, Michigan, United States, 2020-02-14 - 2020-02-14. (LA-UR-20-21574)

Lawrence, E. C., A. Biswas, L. Van Roekel, S. Dutta, L. Tang, S. K. Morley, N. E. Klein, S. Hazarika, M. J. Grosskopf, N. Panda, M. F. Dorn, K. N. Rumsey and D. Banesh. In Situ Inference Project Appraisal. Presented at *In Situ Inference Project Appraisal*, Los Alamos, New Mexico, United States, 2020-12-22 - 2020-12-22. (LA-UR-20-30332)

W. Myren, S. T. In-situ Inference for Exascale Computing. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-04 - 2020-08-04. (LA-UR-20-25683)

Shen, J., S. K. Morley and A. Biswas. Data reduction for large-scale space weather models using machine learning. . (LA-UR-20-26376)

Urban, N. M., A. Biswas, E. C. Lawrence, M. F. Dorn, S. Dutta, M. J. Grosskopf, S. Hazarika, M. G. Henderson, V. K. Jordanova, S. K. Morley, S. T. W. Myren, D. A. Oyen, L. Tang, L. Van Roekel and J. D. Wolfe. In-Situ Inference: Bringing advanced data science into exascale simulations. . (LA-UR-20-23505)

Optimizing Machine Learning for Science and Security

Russell Bent
20200016DR

Project Description

Machine learning (ML) has achieved remarkable successes–becoming a world champion in the Golang (or "Go") programming language, demonstrating super-human video game performance, enabling the advent of self-driving cars, and supporting voice-based personal assistants (e.g., Apple's Siri and Amazon's Alexa). Extending these successes to applications in national security and scientific discovery imposes additional requirements–satisfaction of security constraints and physical laws, robustness to error, and computational tractability–on the next generation of ML innovations. To address these formidable challenges, this work proposes to build on recent advances in large-scale optimization algorithms and enables new ML formulations.

Technical Outcomes

In tractable learning, this project contributed an importance sampling approach that estimates a high-dimensional integral, which can be used to learn failure probabilities of a power system. In constrained and robust learning, the project advanced point cloud alignment and registration by introducing the first rigorous mathematical formulation of the problem. The project devised new algorithms with better accuracy than state-of-the-art techniques based on domain knowledge associated with sensor alignment and noise in the sensors.

Publications

Journal Articles

K. Hari, S. K., A. Nayak and S. Rathinam. An Approximation Algorithm for a Task Allocation, Sequencing and Scheduling Problem Involving a Human-Robot Team. 2020. *IEEE Robotics and Automation Letters*. **5** (2): 2146-2153. (LA-UR-20-21915 DOI: 10.1109/LRA.2020.2970689)

K. Hari, S. K., S. Rathinam, S. Darbha, K. Kalyanam, S. Manyam and D. Casebeer. Optimal UAV Route Planning for Persistent Monitoring Missions. Submitted to *IEEE Transactions on Robotics*. (LA-UR-20-27002)

Misra, S., K. Sundar, R. Sharma and K. Brink. Deployable, Data-Driven Unmanned Vehicle Navigation System in GPS-Denied, Feature-Deficient Environments. Submitted to *IEEE Transactions on Robotics*. (LA-UR-21-20249)

C. Pena Ordieres, A. d., J. LUEDTKE and A. Waechter. SOLVING CHANCE-CONSTRAINED PROBLEMS VIA A SMOOTH SAMPLE-BASED NONLINEAR APPROXIMATION. Submitted to *SIAM Journal on Optimization*. (LA-UR-20-24235)

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Hijazi, H. L., A. M. A. Hijazi, J. B. Dann, A. D. Collins, E. S. Schultz-Fellenz, R. W. Bent and G. Riemersma. ARMO: Alignment and Registration via Mathematical Optimization. Presented at *SIAM International Conference on Data Mining (SDM21)*. (Online, New Mexico, United States, 2021-04-21 - 2021-05-01). (LA-UR-20-28088)

Other

Hijazi, H. L. Anonymized LiDAR Dataset. Dataset. (LA-UR-20-28196)

Effects of Cosmic Ray Neutrons on Modern High Performance Computing (HPC) Components

Nathan Debardeleben
20180017ER

Project Description

Advanced supercomputer systems are using technologies and components of amazing scale and complexity. As we push into these extreme regions, we also greatly push the envelope in the reliability of the systems both in terms of productive use of the machine (utilization, throughput, uptime, etc.) but also in the integrity (correctness) of the calculations done on these systems. It is imperative that we fully understand the causes of interruptions on these extreme-scale systems so that we can better understand how to build and operate them not only for the next generation systems but also the computing industry. Today's extreme-scale supercomputers become tomorrow's corporate supercomputers for technical and economic innovation. To accomplish this, we will use historical data from LANL supercomputers to attribute causes to effects, particularly environmental effects, which are believed to be the primary cause for errors on these systems. Based on preliminary work by the team, we will deploy neutron detectors, correlate the rate with system events, model, and simulate the expected neutron impacts on the supercomputer using advanced software simulation tools. We will also study the effects of solar events (coronal mass ejections) and evaluate the efficacy of shielding the supercomputer from a variety of error sources.

Publications

Journal Articles

Bowen, C. M., N. A. Debardeleben, S. P. Blanchard and C. M. Anderson-Cook. Do Solar Proton Events Reduce the Number of Faults in Supercomputers?: A Comparative Analysis of Faults during and without Solar Proton Events. Submitted to *IEEE International Reliability Physics Symposium*. (LA-UR-19-31047)

Oliveira, D., S. P. Blanchard, N. A. Debardeleben, F. F. dos Santos, G. Piscoya Dávila, P. Navaux, A. Favalli, O. M. Schappert, S. A. Wender, C. Cazzaniga, C. Frost and P. Rech. Thermal Neutrons: a Possible Threat for Supercomputer Reliability. Submitted to *Journal of Supercomputing*. (LA-UR-20-23114)

Conference Papers

Blanchard, S. P., N. A. Debardeleben, P. Rech and D. Oliveira. Thermal Neutrons: A New Threat for Supercomputers and Safety Critical Applications. Presented at *SC'19*. (Denver, Colorado, United States, 2019-11-17 - 2019-11-17). (LA-UR-19-23232)

Oliveira, D., S. P. Blanchard, N. A. Debardeleben, F. F. dos Santos, G. P. D\xc3\xa1vila, P. Navaux, S. A. Wender, C. Cazzaniga, C. Frost, R. Baumann and P. Rech. An Overview of the Risk Posed by Thermal Neutrons to the Reliability of Computing Devices. Presented at *50th IEEE/IFIP Int. Conference on Dependable Systems and Networks*. (Valencia, Spain, 2020-06-29 - 2020-07-02). (LA-UR-20-23268)

Reports

Wender, S. A., A. J. Couture and T. D. Fairbanks. Report on the Tin-II Thermal Neutron Detector. Unpublished report. (LA-UR-19-30822)

Presentation Slides

Bowen, C. M. Telling a Visual Story within Big Data: Case Studies on Interactive Visualizations for Supercomputer Data. Presented at *Rising Stars in Computational and Data Sciences*, Austin, Texas, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-22930)

Bowen, C. M. Telling a visual story within big data: case studies on interactive visualizations for supercomputer data. Presented at *21st Meeting of New Researchers in Statistics and Probability*, Fort Collins, Colorado, United States, 2019-07-24 - 2019-07-24. (LA-UR-19-26857)

Bowen, C. M., N. A. Debardeleben, S. P. Blanchard and C. M. Anderson-Cook. Do Solar Proton Events Reduce the Number of Faults in Supercomputers?: A Comparative Analysis of Faults during and without Solar Proton Events. Presented at *2019 Institute of Electrical and Electronics Engineers International Reliability Physics Symposium*, Monterey, California, United States, 2019-03-31 - 2019-03-31. (LA-UR-19-22250)

R. Mullin, E. R., S. F. Nowicki, N. A. Debardeleben, S. P. Blanchard, S. A. Wender and E. A. Baseman. Pre-deployment Characterization of Large Fast Neutron Detectors for High Performance Computing Fault Characterization. Presented at *2018 Symposium on Radiation Measurements and Applications (SORMA XVII)*, Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-14. (LA-UR-18-21582)

Nowicki, S. F., L. Ferres, E. R. R. Mullin, S. P. Blanchard, N. A. Debardeleben, S. A. Wender and G. E. McMath. Neutron Environment at High-Altitude High-Performance Computing Facilities. Presented at *NSREC*, Santa Fe, New Mexico, United States, 2020-10-30 - 2020-10-30. (LA-UR-20-28797)

Oliveira, D., S. P. Blanchard, N. A. Debardeleben, F. dos Santos, G. Piscoya, P. Navaux, S. A. Wender, C. Cazzaniga, C. Frost, R. Baumann and P. Rech. Thermal Neutrons: a Possible Threat for Supercomputers and Safety Critical Applications. Presented at *SELSE 2020*, Stanford, California, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-23267)

Ortega, S. P., N. A. Debardeleben and C. M. Bowen. Differential Privacy for Supercomputer Sensor Data. Presented at *USRC and HPC Symposia*, Los Alamos, New Mexico, United States, 2019-07-31 - 2019-08-01. (LA-UR-19-27434)

Posters

Bowen, C. M. Telling a Visual Story within Big Data: Case Studies on Interactive Visualizations for Supercomputer Data. Presented at *Spring Research Conference*, Blacksburg, Virginia, United States, 2019-05-22 - 2019-05-22. (LA-UR-19-24529)

Debardeleben, N. A. Data Analytics for Neutron Detection. Presented at *Ultrascale Systems Research Center Research Symposium*, Los Alamos, New Mexico, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-27103)

Ortega, S. P., N. A. Debardeleben and C. M. Bowen. Differential Privacy for Supercomputer Sensor Data. . (LA-UR-19-27097)

Schappert, O. M., S. P. Blanchard, N. A. Debardeleben, R. E. Lakis and A. Favalli. MCNP Simulations of Neutron Fluxes Through Trinity Supercomputer Nodes. . (LA-UR-19-27755)

Massively-Parallel Acceleration of the Dynamics of Complex Systems: a Data-Driven Approach

Danny Perez

20190034ER

Project Description

Current atomistic modeling techniques are limited to extremely short timescales (on the order of microseconds or less), no matter the size of the computer that is used to carry out the simulations. This severely limits their ability to directly interpret experiments or to predict how materials will perform in real life. The key to addressing this problem is to find more efficient ways to exploit the computing power available via the Department of Energy's very large computers. We will develop and implement powerful massively-parallel algorithms deployed on thousands of processors in order to dramatically extend the range of systems that can be simulated over very long times. We will demonstrate the approach on a range of problems of interest to DOE, including the motion of dislocations in materials (materials failure in extreme conditions), the evolution of complex defects in nuclear materials (nuclear safety) and the evolution of bio-molecules (bio-security). In all of these cases, the lack of access to long-times has so far made computational materials design and drug design extremely challenging. Our goal is to use powerful algorithms and very-large-scale computing to directly tackle this challenge.

Publications

Journal Articles

Perez, D., A. Agarwal, A. F. Voter and S. Gnanakaran. Arbitrary accurate representation of atomistic dynamics via semi-Markov jump processes. Submitted to *TBD*. (LA-UR-19-29252)

Perez, D., M. Boleininger, M. Gallauer, S. Dudarev, T. Swinburne and D. Mason. Statistical mechanics of kinks on a gliding screw dislocation. Submitted to *TBD*. (LA-UR-20-23814)

Presentation Slides

Mathew, N., E. Martinez Saez and D. Perez. Accelerated Molecular Dynamics Simulations of Dislocation-Obstacle Interactions in Tungsten: Enabling Micro-Second Simulations. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22073)

Mathew, N., E. Martinez and D. Perez. Investigating Dislocation-Obstacle Interactions in Tungsten using a novel Parallel Replica Dynamics Method. Presented at *APS March Meeting 2021*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22342)

Perez, D. Complex High-Dimensional Energy Landscapes. Presented at *Reunion workshop of the Complex High-Dimensional Energy Landscapes program.*, Lake Arrowhead, California, United States, 2019-06-10 - 2019-06-10. (LA-UR-19-25405)

Objective Flow Topology

Roxana Bujack
20190143ER

Project Description

High Explosives safety and surety and nuclear energy research rely heavily on computational simulations. DOE's supercomputers, expert scientists, and advanced hydrodynamics codes produce ever increasing datasets. This creates new challenges. First, while computational resources are increasing in modern high performance computing (HPC) architectures, the capacity for loading and storing data is not keeping pace- in effect, more data is produced than can be stored. The second problem is that scientists cannot view and comprehend ever larger amounts of flow data during visual analysis because human vision has finite resolution. Our proposed method will solve both problems by providing the means to better analyze big flow data by reducing it to its most essential structure. Firstly, it compresses the data, which helps overcome the Input/Output (I/O) bottleneck and allows the analysis of huge simulation data on a desktop machine with minimal loss of relevant information. Secondly, it produces a decluttered visualization of the fundamental behavior of the flow with minimal occlusion from less important regions.

Publications

Journal Articles

Bujack, R. B., K. C. Tsai, S. K. Morley and E. Brescani. vtkVectorFieldTopology Open Source Topology for 2D and 3D Vector Fields. Submitted to *softwareX*. (LA-UR-20-29277)

*Bujack, R. and A. Middel. State of the art in flow visualization in the environmental sciences. 2020. *Environmental Earth Sciences*. **79** (2): 65. (LA-UR-19-31637 DOI: 10.1007/s12665-019-8800-4)

Conference Papers

Bujack, R. B. Visualization of Distinguished Trajectories as a Generalization of Critical Points to Time-dependent Flow. Presented at *IEEE VIS*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-20-23159)

Bujack, R. B. Comparison of Different Methods to Extract Vector Field Topology on Finite Domains. Presented at *IEEE VIS*. (New Orleans, Louisiana, United States, 2021-10-24 - 2021-10-24). (LA-UR-21-20582)

Bujack, R. B., E. Bresciani, J. Waters and W. Schroeder. Topological Segmentation of 2D Vector Fields. Presented at *EnvirVis*. (Zurich, Switzerland, 2021-06-14 - 2021-06-14). (LA-UR-21-21785)

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. Time-Dependent Flow Topology: Past, Present, and Future. Presented at *EuroVis*. (Lingkoeping, Sweden, 2020-06-03 - 2020-06-03). (LA-UR-19-30267)

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. State of the Art in Time-Dependent Flow Topology: Interpreting Physical Meaningfulness Through Mathematical Properties. Presented at *EuroVis*. (Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25). (LA-UR-20-23019)

Bujack, R. B., S. Dutta, D. Z. Zhang and T. Gunther. Objective Finite-Time Flow Topology from Flowmap Expansion and Contraction. Presented at *TopoInVis*. (Nyk\xc3\xb6ping, Sweden, 2019-06-17 - 2019-06-19). (LA-UR-19-23386)

Bujack, R. B., S. Dutta, I. B. Rojo, D. Z. Zhang and T. G \xc3\xbcnther. Objective Finite-Time Saddles and their Connection to FTLE. Presented at *EuroVis 2019*. (Porto, Portugal, 2019-06-03 - 2019-06-07). (LA-UR-19-21831)

Bujack, R. B., S. Sane, C. Garth and H. Childs. Survey of Seed Placement and Streamline Selection Techniques. Presented at *EuroVis*. (Linkoeping, Sweden, 2019-06-03 - 2019-06-03). (LA-UR-19-30263)

Dutta, S., R. X. Brady, M. E. Maltrud, P. J. J. Wolfram and R. B. Bujack. Leveraging Lagrangian Analysis for Discriminating Nutrient Origins. Presented at *Visualization in Environmental Sciences*. (Porto, Portugal, 2019-06-03 - 2019-06-03). (LA-UR-19-22455)

Yan, L., B. Wang and R. B. Bujack. Finite-time Saddles from Particle Origin and Destination. Presented at *Eurovis 2020*. (Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25). (LA-UR-19-26219)

Books/Chapters

Bujack, R. B. Mathematical Foundations in Visualization. (LA-UR-19-29121)

Reports

Bujack, R. B. The Definition of a Separatrix. Unpublished report. (LA-UR-21-22238)

Presentation Slides

Bujack, R. B. State of the Art in Time-Dependent Flow Topology: Interpreting Physical Meaningfulness Through Mathematical Properties. Presented at *EuroVis*, Norrk \xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25. (LA-UR-20-23457)

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. State of the Art in Time-Dependent Flow Topology: Interpreting Physical Meaningfulness Through Mathematical Properties. Presented at *EuroVis*, Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25. (LA-UR-20-23456)

Towards Memristor Supremacy with Novel Machine Learning Algorithms

Francesco Caravelli
20190195ER

Project Description

Memristors are the nanoscale equivalent of brain synapses: these are passive components able to learn, and their prospective application is in reproducing the capabilities of the brain. This project is a first step towards the integration of (hard) computational tasks in dense nanoscale analog circuits. The success of this project will show that the use of memristors without a complementary metal oxide semiconductor (CMOS), the base for current computational architectures, can still be used for storage and low-energy computation. The addition of CMOS hardware will then be used for hybrid brain-like and digital-like computers. This project is aligned with the goal of "Beyond Moore's Law" computation, one the Department of Energy missions. While some brain-like chips are currently available, their architecture is simple; the purpose of this project is to go beyond standard architectures.

Publications

Journal Articles

*Caravelli, F. Asymptotic Behavior of Memristive Circuits. 2019. *Entropy*. **21** (8): 789. (LA-UR-18-24748 DOI: 10.3390/e21080789)

Caravelli, F. Inversion-free Leontief inverse: statistical regularities in input-output analysis from partial information. Submitted to *Revista Mexicana de Fisica*. (LA-UR-20-26892)

Caravelli, F., C. Nisoli and G. Chern. Phase-change spin ice memory resistor. Submitted to *Physical Review Letters*. (LA-UR-19-27438)

Caravelli, F., F. C. Sheldon and F. L. Traversa. Tunneling through barrier by passive dynamical system. Submitted to *Physical Review Letters*. (LA-UR-20-28084)

Caravelli, F., F. C. Sheldon and F. L. Traversa. Global minimization via classical tunneling assisted by collective force field formation. Submitted to *Nature Physics*. (LA-UR-21-20810)

Caravelli, F., S. Bartolucci, F. Caccioli and P. Vivo. Universal Rankings in complex input-output organizations. Submitted to *Nature*. (LA-UR-20-27058)

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

*Caravelli, F. and J. P. Carbajal. Memristors for the Curious Outsiders. 2018. *Technologies*. **6** (4): 118. (LA-UR-18-27766 DOI: 10.3390/technologies6040118)

Pang, Y., C. J. Coffrin, A. Lokhov and M. D. Vuffray. The potential of quantum annealing for rapid solution structure identification. 2020. *Constraints*. (LA-UR-20-22733 DOI: 10.1007/s10601-020-09315-0)

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)

Sheldon, F. C., F. Caravelli and A. Kolchinsky. The Computational Capacity of Memristor Reservoirs. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-26991)

*Zegarac, A. and F. Caravelli. Memristive networks: From graph theory to statistical physics. 2019. *EPL (Europhysics Letters)*. **125** (1): 10001. (LA-UR-18-31372 DOI: 10.1209/0295-5075/125/10001)

Conference Papers

Coffrin, C. J., H. Nagarajan and R. W. Bent. Evaluating Ising Processing Units with Integer Programming. Presented at *Sixteenth International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Thessaloniki, Greece, 2019-06-04 - 2019-06-07). (LA-UR-19-22000)

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)

Jayakumar, A., A. Lokhov, S. Misra and M. D. Vuffray. Learning of Discrete Graphical Models with Neural Networks.

Presented at *NeurIPS*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-24927)

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)

Pang, Y., C. J. Coffrin, A. Lokhov and M. D. Vuffray. The Potential of Quantum Annealing for Rapid Solution Structure Identification. Presented at *17th International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Vienna, Austria, 2020-05-26 - 2020-05-29). (LA-UR-19-31884)

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *COLT 2019 : Computational Learning Theory*. (Phoenix, Arizona, United States, 2019-06-25 - 2019-06-29). (LA-UR-19-20925)

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)

Books/Chapters

Sheldon, F. C., C. J. Coffrin and F. Caravelli. Fully analog memristive circuits for optimization tasks: a comparison. (LA-UR-20-26683)

Presentation Slides

Caravelli, F. Memristive Networks. Presented at *Talk @ICTP Trieste*, Trieste, Italy, 2019-09-23 - 2019-09-23. (LA-UR-19-29539)

Caravelli, F. Computing with memristive devices and networks. . (LA-UR-20-29385)

Coffrin, C. J. Beyond Moore's Law: Exploring the Future of Computation. . (LA-UR-19-21268)

Coffrin, C. J. Novel Computing Platforms: Potential and Challenges for Discrete Optimization. . (LA-UR-19-21267)

Coffrin, C. J. Challenges with Chains: Testing the Limits of a D-Wave Quantum Annealer for Discrete Optimization. . (LA-UR-19-21739)

Coffrin, C. J. Harnessing Analog Noise: A Hybrid Algorithm for Binary Quadratic Optimization with Uncertainty. . (LA-UR-19-24684)

Coffrin, C. J. The Potential of Quantum Annealing for Rapid Solution Structure Identification. . (LA-UR-20-21046)

Lokhov, A. Uncovering the behavior of quantum annealers with statistical learning. Presented at *APS march meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-22165)

Lokhov, A. Uncovering the behavior of quantum annealers with statistical learning. Presented at *At the crossroads of physics and machine learning*, Santa Barbara, California, United States, 2019-02-11 - 2019-02-11. (LA-UR-19-22163)

Lokhov, A. Learning Discrete Graphical Models with Neural Networks. Presented at *Youth in High-dimensions: Machine Learning, High-dimensional Statistics and Inference for the New Generation*, Online, New Mexico, United States, 2020-06-29 - 2020-06-29. (LA-UR-20-24925)

Lokhov, A. Learning of Discrete Graphical Models: Ising, Potts, and beyond. Presented at *Statistical mechanics methods for networks*, Online, New Mexico, United States, 2020-09-17 - 2020-09-17. (LA-UR-20-27372)

Sheldon, F. C., A. Kolchinsky and F. Caravelli. The Computational Capacity of Mem-LRC Networks. Presented at *NICE*, NICE, Germany, 2021-03-09 - 2021-03-09. (LA-UR-21-22337)

Vuffray, M. D., S. Misra and A. Lokhov. Learning Discrete Graphical Models Exact & Neural Assisted Methods. Presented at *IMA: Theory and Algorithms in Graph-based Learning workshop*, Mineapolis, Minnesota, United States, 2020-09-14 - 2020-09-18. (LA-UR-20-27337)

Posters

Lokhov, A. Optimal deployment of resources for maximizing impact in spreading processes. Presented at *APS march meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-22164)

Other

Coffrin, C. J. The Potential of Quantum Annealing for Rapid Solution Structure Identification (video). Audio/Visual. (LA-UR-20-23778)

Stable, Conservative, High-Order Numerical Methods for Direct Numerical Simulations (DNS) in Complex Geometries

Peter Brady
20190227ER

Project Description

Numerical simulations play a key role in stockpile stewardship. The large scale industrial simulations that are required for understanding the complex regimes arising from stockpile stewardship considerations employ a variety simplified physical models. The development and assessment of these models can be greatly enhanced by reliable databases produced by more focused, high-fidelity simulations. This project will extend the capabilities of high-fidelity, exa-scale simulations to the complex configurations that are typically encountered in engineering applications.

Publications

Journal Articles

Brady, P. T. and D. Livescu. Foundations for high-order, conservative cut-cell methods: Stable discretizations on degenerate meshes. 2020. *Journal of Computational Physics*. 109794. (LA-UR-20-22279 DOI: 10.1016/j.jcp.2020.109794)

Sharan, N., P. T. Brady and D. Livescu. Time-stable strong boundary conditions in finite-difference schemes for hyperbolic systems. Submitted to *Journal of Computational Physics*. (LA-UR-20-24938)

Conference Papers

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-Cell Methods. Presented at *AIAA Scitech*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-29984)

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-Cell Methods. Presented at *AIAA SciTech Forum*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-31402)

Sharan, N., P. T. Brady and D. Livescu. Stable and conservative boundary treatment for difference methods, with application to cut-cell discretizations. Presented at *2020 AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-32707)

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. Numerical Study of the Properties of a Ghost-Cell Method. Presented at *American Institute of Aeronautics and Astronautics*. (Orlando, Florida, United States, 2020-01-07 - 2020-01-11). (LA-UR-19-28614)

Reports

Brady, P. T. and D. Livescu. High-Order, Stable, and Conservative Boundary Schemes for Central and Compact Finite Differences. Unpublished report. (LA-UR-19-20056)

Presentation Slides

Brady, P. T. and D. Livescu. A Foundation for High-Order Cut-Cell Methods: Stable Derivatives on Degenerate Meshes. Presented at *APS DFD*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-30896)

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-cell Methods. Presented at *AIAA Scitech*, San Diego, California, United States, 2019-01-07 - 2019-01-07. (LA-UR-19-20057)

Brady, P. T. and D. Livescu. High-Order Cut-Cell Methods in Multiple Dimensions. Presented at *72nd APS DFD meeting*, Seattle, Washington, United States, 2019-11-23 - 2019-11-23. (LA-UR-19-31797)

Kim, K. H. Composition and Dynamical Processes of Ions in Giant Magnetospheres: The Importance of In Situ Measurements for Advancing the Current Knowledge. . (LA-UR-20-28874)

Sharan, N., P. T. Brady and D. Livescu. High-order energy-stable boundary treatment for finite-difference cut-cell method. Presented at *72nd Annual Meeting of the APS Division of Fluid Dynamics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31665)

Sharan, N., P. T. Brady and D. Livescu. Stable and conservative boundary treatment for difference methods, with application to cut-cell discretizations. Presented at *2020 AIAA SciTech Forum*, Orlando, Florida, United States, 2020-01-06 - 2020-01-06. (LA-UR-20-20086)

Sharan, N., P. T. Brady and D. Livescu. Dimensionally-split provably stable cut-cell approach for flow calculations. Presented at *APS Division of Fluid Dynamics Meeting*

2020, Online, New Mexico, United States, 2020-11-22 - 2020-11-24. (LA-UR-20-29646)

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. High-Order Ghost-Cell Method for Non-Conforming Boundaries. Presented at *American Physical Society Division of Fluid Dynamics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31645)

Posters

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. High-Order Ghost-Point Method for Non-Conforming Boundaries. Presented at *Los Alamos Post-doc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28565)

Statistical Learning in Cyberphysical Systems

Nathan Lemons
20190351ER

Project Description

The overarching goal of this project is to develop novel data-driven algorithms for statisical learning of an effective high-fidelity representation of cyberphysical systems. This will allow applications such as real-time detection and classification of anomalies, state estimation for damage-recovery operations, and optimal expansion of the system. We expect our work to be highly relevant to those tasked with operating and protecting large networked cyberphysical systems, such as electric grids. This research is directly relevant to the program office "Cybersecurity for Energy Delivery Systems" within the Office of Electricity in the Department of Energy. It is expected that members of the Intelligence Community will also be interested in this work. We also expect to contribute to the state of the art in machine learning and statistical learning through publications and presentations at top conferences.

Publications

Journal Articles

Balogh, J., N. W. Lemons and C. Palmer. Maximum size intersecting families of bounded minimum positive co-degree. Submitted to *Electronic Journal of Combinatorics*. (LA-UR-20-23462)

Chertkov, M., V. Y. Chernyak and Y. Maximov. Gauges, Loops, and Polynomials for Partition Functions of Graphical Models. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-20-30432)

Gy\xc5\x91ri, E., N. W. Lemons, N. Salia and O. Zamora. The structure of hypergraphs without long Berge cycles. 2020. *Electronic Journal of Combinatorics*. (LA-UR-18-31512 DOI: 10.1016/j.jctb.2020.04.007)

Keszegh, B., N. W. Lemons, R. R. Martin, D. P\xc3\xa1lv \xc3\xb6lgyi and B. Patk\xc3\xb3s. Induced and non-induced poset saturation problems. Submitted to *SIAM Journal on Discrete Mathematics*. (LA-UR-20-22232)

Lemons, D. S., N. W. Lemons and W. Peter. Benford's Law and the Unbiased Sparse Partitioning of a Conserved Quantity. Submitted to *Physical Review E*. (LA-UR-20-23463)

Likhosherstov, V., Y. Maximov and M. Chertkov. Tractable Minor-free Generalization of Planar Zero-field Ising Models. Submitted to *IEEE Transactions on Information Theory*. (LA-UR-19-30102)

Oles, V., N. W. Lemons and A. Panchenko. EFFICIENT ESTIMATION OF A GROMOV–HAUSDORFF DISTANCE BETWEEN UNWEIGHTED GRAPHS. Submitted to *IEEE Transactions on Pattern Analysis and Machine Intelligence*. (LA-UR-19-28284)

Conference Papers

Deka, D., U. Hashmi, L. Pereira, A. Busic and S. N. Backhaus. Co-optimizing Energy Storage for Prosumers using Convex Relaxations. Presented at *ISAP Conference 2019*. (New Delhi, India, 2019-12-10 - 2019-12-14). (LA-UR-19-29297)

Deka, D. and S. Misra. Learning for DC-OPF: Classifying active sets using neural nets. Presented at *Powertech 2019*. (milan, Italy, 2019-06-23 - 2019-06-27). (LA-UR-19-24726)

Hannon, C. M., D. Deka, D. Jin, M. D. Vuffray and A. Lokhov. Real-time Anomaly Detection and Classification in Streaming PMU Data. Presented at *XXI Power Systems Computation Conference*. (Porto, Portugal, 2020-06-29 - 2020-07-03). (LA-UR-19-31329)

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)

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *COLT 2019 : Computational Learning Theory*. (Phoenix, Arizona, United States, 2019-06-25 - 2019-06-29). (LA-UR-19-20925)

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

Belyy, A., A. Sholokhov, M. R. Amini and Y. Maximov. MEMOIR: Multi-class Extreme Classification with Inexact Margin. Unpublished report. (LA-UR-19-21219)

Burashnikova, A., Y. Maximov and M. R. Amini. Sequential Learning over Implicit Feedback for Robust Large-Scale Recommender Systems. Unpublished report. (LA-UR-19-21349)

Krechetov, M., Y. Maximov, J. Marecek and M. Takac. Entropy-Penalized Semidefinite Programming. Unpublished report. (LA-UR-18-24430)

Likhosherstov, V., Y. Maximov and M. Chertkov. Inference and Sampling of K33-free Ising Models. Unpublished report. (LA-UR-19-26932)

Likhosherstov, V., Y. Maximov and M. Chertkov. A New Family of Tractable Ising Models. Unpublished report. (LA-UR-19-24712)

Maximov, Y., A. Burashnikova, N. Dante, M. Clausel, M. R. Amini and R. Stoica. Recommender systems : when memory matters. Unpublished report. (LA-UR-21-22659)

Presentation Slides

Deka, D., H. Doddi and A. Lokhov. Sample Optimal topology learning of linear dynamical systems. . (LA-UR-20-25926)

Hannon, C. M., D. Deka, M. D. Vuffray and A. Lokhov. Real-time Modeling and Anomaly Detection in Cyber-physical Systems. . (LA-UR-20-22487)

Lemons, N. W. Statistical Learning in Cyberphysical Systems. . (LA-UR-21-20316)

Lokhov, A. Learning Discrete Graphical Models with Neural Networks. Presented at *Youth in High-dimensions: Machine Learning, High-dimensional Statistics and Inference for the New Generation*, Online, New Mexico, United States, 2020-06-29 - 2020-06-29. (LA-UR-20-24925)

Lokhov, A. Learning of Discrete Graphical Models: Ising, Potts, and beyond. Presented at *Statistical mechanics methods for networks*, Online, New Mexico, United States, 2020-09-17 - 2020-09-17. (LA-UR-20-27372)

Posters

Hannon, C., D. Deka and A. Lokhov. Realtime Modeling and Anomaly Detection in Cyber-Physical Systems. Presented at *NeurIPS*, Los Alamos, New Mexico, United States, 2019-12-08 - 2019-12-14. (LA-UR-19-32246)

Quantum Computing with Strontium Nuclear Qubits

Michael Martin
20200015ER

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.

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)

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)

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. 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)

Topological Relation-Based Image Analysis using Graphs

Diane Oyen
20200041ER

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.

Publications

Conference Papers

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. 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)

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)

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)

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)

Adaptive High-order Finite Element Arbitrary Lagrangian-Eulerian (ALE) Methods for Multi-material Hydrodynamics

Jacob Waltz
20200201ER

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.

Publications

Journal Articles

Pandare, A. K., J. I. Waltz and J. Bakosi. Multi-Material Hydrodynamics with Algebraic Sharp Interface Capturing. 2020. *Computers & Fluids*. 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)

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)

Sampling the Unknown: Robust Modeling of Atomic Potentials

Kipton Barros
20200209ER

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.

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)

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)

Sifain, A. E., L. A. Lystrom, R. A. Messerly, J. S. Smith, B. T. Nebgen, K. M. Barros, S. Tretiak, N. E. Lubbers and B. J. Gifford. Predicting Phosphorescence and Inferring Wavefunction Localization with Machine Learning. Submitted to *Chemical Science*. (LA-UR-21-21632)

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., 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)

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. and J. S. Smith. Midterm LDRD Appraisal 20200209ER. . (LA-UR-20-29553)

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)

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)

Unlocking the Power of Tensor Cores with Mixed Precision Algorithms

Anders Niklasson
20200225ER

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.

Publications

Journal Articles

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)

Dielectric Antenna Array for Pinpoint Data/Energy Targeting

John Singleton
20200285ER

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.

Publications

Journal Articles

Schmidt, A. C., C. Bailey, F. L. Krawczyk, J. M. Wigger and J. Singleton. On the information carried by electromagnetic radiation launched from accelerated polarization currents. Submitted to *Journal of Applied Physics*. (LA-UR-20-23902)

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)

Enabling Fast Disaggregation of Large Parameter Spaces

Kary Myers
20180097ER

Project Description

We propose an entirely new way to address the fundamental scientific goal of disaggregation, or estimation of the components of an unknown measured target. Disaggregation problems appear in national security problems such as nuclear forensics and power grid analysis. Our approach combines forward models with measurements to estimate a target's component proportions while accounting for uncertainty. This work will advance both computer model calibration (to make disaggregation possible) and emulation (to make disaggregation fast). Compared to a brute force approach that can require a year of computation to estimate a single target's composition, our strategy will create a fast estimation procedure that could ultimately support processing of data on board a sensor.

Technical Outcomes

This project developed methodology for disaggregation of laser-induced breakdown spectra. The approach incorporates physics knowledge to emulate a forward model in a way that circumvents the need to explore all combinations of elemental components. This allows us to quickly estimate the abundance of the elemental components in a given sample. This work also includes estimation of systematic differences between the model and data and a new approach to dimension reduction for building emulators with non-linear variation.

Publications

Journal Articles

Bhat, K. G., K. L. Myers, E. C. Lawrence, J. P. Colgan and E. Judge. Using computer model calibration to estimate instrument response parameters. Submitted to *Technometrics*. (LA-UR-19-22659)

Bhat, K. G., K. L. Myers, E. C. Lawrence, J. P. Colgan and E. Judge. Physics informed composite emulation for laser-induced breakdown spectroscopy. Submitted to *Annals of Applied Statistics*. (LA-UR-20-27637)

C. Hebert, C. M., E. C. Lawrence, K. L. Myers, K. G. Bhat, J. P. Colgan and E. Judge. Non-negative matrix factorization for Modular Bayesian calibration of plasma compositions. Submitted to *Journal of the American Statistical Association*. (LA-UR-19-30403)

Hebert, C., E. C. Lawrence, K. L. Myers and J. P. Colgan. Modular Bayesian calibration for plasma composition. Submitted to *Statistical Analysis and Data Mining*. (LA-UR-20-25226)

Klein, N. E., E. C. Lawrence and K. L. Myers. Deep autoencoder neural networks for dimension reduction in Gaussian process model calibration. Submitted to *SIAM/ASA Journal on Uncertainty Quantification*. (LA-UR-20-27282)

Presentation Slides

Bhat, K. G. Science-based Statistical Characterization of Matrix Effects. . (LA-UR-20-25884)

C. Hebert, C. M. Rocky beginnings: emulation for ChemCam data analysis. . (LA-UR-18-30744)

C. Hebert, C. M., K. L. Myers and E. C. Lawrence. Emulation for ChemCam data analysis. . (LA-UR-18-30784)

Klein, N. E. A statistics journey to Mars!. Presented at *UNM Graduate Statistics Club*, Albuquerque, New Mexico, United States, 2019-12-06 - 2019-12-06. (LA-UR-19-31807)

Klein, N. E., E. C. Lawrence, K. L. Myers, E. Judge and J. P. Colgan. Is There ____ on Mars?: Disaggregation of LIBS Spectra. Presented at *Joint Statistical Meetings 2020*, Online, New Mexico, United States, 2020-08-01 - 2020-08-06. (LA-UR-20-25422)

Lawrence, E. C. Computer Experiments at Los Alamos National Laboratory: Life on Mars and Really Big Computers. Presented at *The University of Michigan Department of Statistics Distinguished Alumni Speaker Series*, Ann Arbor, Michigan, United States, 2020-02-14 - 2020-02-14. (LA-UR-20-21574)

Lawrence, E. C., K. G. Bhat, N. E. Klein, C. Hebert, J. P. Colgan, E. Judge and K. L. Myers. Mars Attacked! Simulation-Based Disaggregation of LIBS Spectra. Presented at *Advanced Statistics meets Machine Learning-III*, Lemont, Illinois, United States, 2019-11-14 - 2019-11-14. (LA-UR-19-31457)

Myers, K. L., K. G. Bhat, E. C. Lawrence, E. Judge, J. P. Colgan and C. M. C. Hebert. Enabling Fast Disaggregation of Large Parameter Spaces. . (LA-UR-18-31077)

Myers, K. L., K. G. Bhat, J. P. Colgan and E. Judge. New Directions in Computer Model Calibration to Enable Disaggregation of Large Parameter Spaces. . (LA-UR-20-25962)

Posters

Bhat, K. G. Multi-Scale Uncertainty Quantification in the Physical Sciences and Engineering for Complex Models. Presented at *Joint Statistical Meetings*, Vancouver, Canada, 2018-07-29 - 2018-08-02. (LA-UR-18-26895)

Bhat, K. G., K. L. Myers, E. C. Lawrence, J. P. Colgan and E. Judge. Multi-Stage Emulation and Uncertainty Quantification for Disaggregation of LIBS Spectra. Presented at *Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21837)

Klein, N. E., E. C. Lawrence, K. L. Myers, J. P. Colgan and E. Judge. Is there ___ on Mars?: Disaggregation of LIBS spectra. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21301)

Other

Colgan, J. P., E. Judge, K. G. Bhat, K. L. Myers and E. C. Lawrence. ATOMIC Simulations and Experimental Data for Sodium and Copper Mixtures. Dataset. (LA-UR-20-23189)

Colgan, J. P., E. Judge, K. G. Bhat, K. L. Myers and E. C. Lawrence. ATOMIC Simulations and Experimental Data for CaCO_3 Mixture. Dataset. (LA-UR-20-30305)

Klein, N. E., K. G. Bhat, K. L. Myers, E. C. Lawrence, E. Judge and J. P. Colgan. ATOMIC Simulations and Experimental Data for Basalt-like Compounds. Dataset. (LA-UR-20-27924)

Synthesizing Fokker-Planck and Navier-Stokes Methods for Strongly Coupled Hydrodynamics and Material Fields in Turbulent Mixing

Raymond Ristorcelli
20180154ER

Project Description

The project develops a new statistical/engineering treatment of the coupled physics of hydrodynamics and turbulent mixing, involving materials with very different properties, e.g., gaseous iron and hydrogen. This requires approximations for problems where the numerical resolution of all relevant physical scales is not economical. We do this by ensuring mathematical and statistical constraints and thus enforce physical realizability constraints, required for correctness and code stability. We anticipate an impact on multiple Los Alamos National Laboratory and DOE/NNSA programs, including high-energy-density hydrodynamics, global security, astrophysics, as well as atmospheric, climate, and fusion energy sciences.

Technical Outcomes

Results of this project include: The development of a new hypothesis testing method for turbulent transport in variable-density turbulence; a joint velocity-species Fokker-Planck strategy for the computation of a joint PDF method for variable-density turbulence; and the development of models for the prediction of turbulent transport in the second moment equations for binary mixing in variable-density turbulence.

Publications

Reports

Ristorcelli, R. and J. Bakosi. A joint Fokker-Planck PDF method for rigorous hypothesis testing of turbulent transport models in variable-density turbulence. Unpublished report. (LA-UR-20-27738)

Hamiltonian on Demand for Computational Materials Using Machine Learning

Sergei Tretiak
20180213ER

Project Description

Computational materials methods have become an indispensable counterpart of experiments. To overcome our current limitations we will construct Machine Learning based algorithms for producing effective Hamiltonian parameters for molecular materials. The developed scalable, general (applicable to any molecular or material system), transferrable and robust algorithms will be able to predict an assortment of quantum mechanical properties of a system with quantitative accuracy. The range of materials include organic semiconductors, bio-molecules, transition metals, actinides and lanthanides. Success in predicting properties of such materials will strongly contribute to the Lab core missions and will provide new capabilities in a range of DOE Office of Science targets.

Technical Outcomes

The project completed the "HIPPYNN" neural network and "PYSEQM" semi-empirical package, which combined can produce customized Hamiltonian parameters for a variety of systems, including biomolecules, organics, and metals. The software efficiently uses Graphical Processing Unit architectures to make quantitative predictions of electronic properties, with the methodology being transferable across wide swaths of chemical space, including proteins. Finally, follow on funding through the Advanced Technology Development and Mitigation (ATDM) program was granted to pursue automated generation of metal potentials on the Sierra supercomputer.

Publications

Journal Articles

*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)

*Kidwell, N. M., B. Nebgen, L. V. Slipchenko and T. S. Zwier. The effects of site asymmetry on near-degenerate state-to-state vibronic mixing in flexible bichromophores. 2019. *The Journal of Chemical Physics*. **151** (8): 084313. (LA-UR-19-29710 DOI: 10.1063/1.5107423)

Magedov, S. I., C. F. Koh, W. F. I. Malone, N. E. Lubbers and B. T. Nebgen. Bond Order Predictions Using Deep Neural Networks. Submitted to *Journal of Applied Physics*. (LA-UR-20-26468)

Nelson, T. R., B. T. Nebgen, A. J. White, Y. Zhang, H. Song, J. A. Bjorgaard, A. E. Sifain, B. Rodriguez-Hernandez, V. M. Freixas, S. Fernandez-Alberti, A. Roitberg, W. F. I. Malone and S. Tretiak. NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22362)

Nelson, T. R., V. M. Freixas, D. Ondarse-Alvarez, P. Nijjar, A. Mikhailovsky, C. Zhou, S. Fernandez-Alberti, G. C. Bazan and S. Tretiak. Experimental and Theoretical Study of Energy Transfer in a Chromophore Triad: What Makes Modeling Dynamics Successful?. Submitted to *Journal of Chemical Physics*. (LA-UR-20-23551)

Rodriguez-Hernandez, B., T. R. Nelson, N. Oldani, A. Martinez-Mesa, L. Uranga-Pina, Y. Segawa, S. Tretiak, K. Itami and S. Fernandez-Alberti. Exciton spatial dynamics and self-trapping in carbon nanocages. Submitted to *Journal of Physical Chemistry A*. (LA-UR-20-29357)

Sifain, A. E., L. A. Lystrom, R. A. Messerly, J. S. Smith, B. T. Nebgen, K. M. Barros, S. Tretiak, N. E. Lubbers and B. J. Gifford. Predicting Phosphorescence and Inferring Wavefunction Localization with Machine Learning. Submitted to *Chemical Science*. (LA-UR-21-21632)

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Presentation Slides

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Lubbers, N. E. Adapting Neural Networks to Atomistic Systems for End-to-End Learning. Presented at *SIAM Conference on Computational Science and Engineering (CSE21)*, Fort Worth, Texas, United States, 2021-03-01 - 2021-03-05. (LA-UR-21-22108)

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Nebgen, B. T., J. S. Smith, N. E. Lubbers, A. E. Sifain, K. M. Barros and S. Tretiak. Machines Learning Quantum Chemistry: Potentials, Properties, and P-Orbitals. Presented at *Telluride workshop: Multi-scale quantum mechanical analysis of condensed phase systems: methods and applications*, Telluride, Colorado, United States, 2018-07-23 - 2018-07-27. (LA-UR-18-26999)

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Nebgen, B. T., N. E. Lubbers and S. Tretiak. Machines learning physics: deep tensor neural networks for dynamically optimized effective Hamiltonians. Presented at *ACS Boston*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-28121)

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Tretiak, S. Modeling of Electronic Properties in Organic and Hybrid Materials. . (LA-UR-19-28826)

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Zhou, G., B. T. Nebgen, N. E. Lubbers and S. Tretiak. Machine Learning with Domain Knowledge of Quantum Chemistry. Presented at *2020 CINT Annual Meeting*, Los Alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27710)

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Magedov, S. I., B. T. Nebgen, N. E. Lubbers, K. M. Barros and S. Tretiak. Prediction of bond orders using deep neural networks. Presented at *Meeting of the American Physical Society*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23861)

Nebgen, B. T., N. E. Lubbers, J. S. Smith, R. Zubatiuk, A. Lokhov, O. Isayev, K. M. Barros and S. Tretiak. Machine Learning For Quantitative H\xc3\xbcckel Theory. Presented at *Excited State Processes*, Santa Fe, New Mexico, United States, 2018-06-03 - 2018-06-07. (LA-UR-18-24826)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, T. C. Germann, S. J. Fensin and K. M. Barros. Discovering physics from disorder: active learning a robust potential for aluminum. . (LA-UR-19-32169)

Preprocessing Algorithms for Boosting Quantum Annealing Scalability

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Project Description

Quantum annealing is recognized by many in the scientific community as one of the promising exascale and "beyond Moore's law" computing technologies. While there are commercially available quantum annealing computers by D-Wave that currently have as many as 2048 quantum bits (qubits), significant innovative research is needed before such computers demonstrate quantum supremacy and become a viable alternative. Taking advantage of the D-Wave 2X computer available at Los Alamos National Laboratory and the expertise of the project team in solving optimization problems using D-Wave, this project addresses some of the biggest challenges to ultimately improve the efficiency and accuracy of quantum annealing computers.

Technical Outcomes

This project developed methods that allow significantly increasing the sizes of the problems that can be solved to optimality on existing quantum annealers by reducing large problems into subproblems, small enough to fit the hardware. The team also optimized the accuracy of the annealer by identifying combinations of tunable hardware parameters that reduce the effects of biases and noise in the hardware.

Publications

Journal Articles

Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihal\xc3\xa1k. Near-gathering of energy-constrained mobile agents. 2020. *Theoretical Computer Science*. (LA-UR-19-23906 DOI: 10.1016/j.tcs.2020.10.008)

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Pakin, S. D. and S. P. Reinhardt. Programming a D-Wave Annealing-Based Quantum Computer: Tools and Techniques. Submitted to *Quantum Information & Computation*. (LA-UR-19-20660)

R. Pelofske, E. A., H. N. Djidjev and G. Hahn. Inferring the Dynamics of Ground-State Evolution of Quantum Annealers. Submitted to *Special Section on Parallel and Distributed Computing Techniques for Non-Von Neumann Technologies*. (LA-UR-20-27022)

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Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Solving large Maximum Clique problems on a quantum annealer. Presented at *First International Workshop on Quantum Technology and Optimization Problems (QTOP'19)*. (Munich, Germany, 2019-03-18 - 2019-03-18). (LA-UR-18-30973)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Advanced anneal paths for improved quantum annealing. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Denver, Colorado, United States, 2020-10-12 - 2020-10-12). (LA-UR-20-23828)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Advanced unembedding techniques for quantum annealers. Presented at *IEEE International Conference on Rebooting*

Computing. (Virtual Conference, New Mexico, United States, 2020-12-01 - 2020-12-03). (LA-UR-20-26972)

Djidjev, H. N., T. Vyskocil and S. D. Pakin. Embedding inequality constraints for quantum annealing optimization. Presented at *First International Workshop on Quantum Technology and Optimization Problems (QTOP'19)*. (Munich, Germany, 2019-03-18 - 2019-03-18). (LA-UR-18-30972)

Djidjev, H. N. and T. Vyskocil. Simple constraint embedding for quantum annealers. Presented at *International Conference on Rebooting Computing*. (Washington, District Of Columbia, United States, 2018-11-07 - 2018-11-07). (LA-UR-18-24168)

Djidjev, H. N. and T. Vyskocil. Optimization approach to constraint embedding for quantum annealers. Presented at *Integer Programming and Combinatorial Optimization*. (Ann Arbor, Michigan, United States, 2019-05-22 - 2019-05-22). (LA-UR-18-30971)

Djidjev, H. N. and T. Vyskocil. Implementing constraints for quantum annealing optimization using finite state automata. Presented at *25th International Computing and Combinatorics Conference (COCOON)*. (Xian, China, 2019-07-29 - 2019-07-29). (LA-UR-19-22730)

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Presentation Slides

Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihal\xc3\xa1k. Near-gathering of energy-constrained mobile agents. Presented at *26th International Colloquium on Structural Information and Communication Complexity SIROCCO 2019*, L'Aquila, Italy, 2019-07-01 - 2019-07-04. (LA-UR-20-22307)

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Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Exploiting some advanced annealing options of the D-Wave 2000Q quantum annealer. Presented at *Qubits Worldwide Users Conference*, Virtual Conference, New Mexico, United States, 2020-09-28 - 2020-09-28. (LA-UR-20-27120)

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Francois, S., R. Andonov and H. N. Djidjev. Assembly of Chloroplast Genomes Using Global Optimization. Presented at *13th Annual Sequencing, Finishing, and Analysis in the Future (SFAF) Conference*, Santa Fe, New Mexico, United States, 2018-05-22 - 2018-05-22. (LA-UR-18-24468)

Pakin, S. D. Targeting Classical Code to a Quantum Annealer. Presented at *24th ACM International Conference on Architectural Support for Programming Languages and Operating Systems*, Providence, Rhode Island, United States, 2019-04-13 - 2019-04-17. (LA-UR-19-23060)

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Chimera and Pegasus Connection Topologies. Presented at *ISC High Performance*, Digital Event, Germany, 2020-06-22 - 2020-06-25. (LA-UR-20-24300)

Posters

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Decomposition Algorithms for Scalable Quantum Annealing. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26700)

Other

Pakin, S. D. and E. G. Rieffel. Tutorial Promotion: Introduction to Quantum Computing. Audio/Visual. (LA-UR-18-28216)

Threat Quantity Indication of Special Nuclear Material

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Project Description

This project will create a real-time threat-identification algorithm that utilizes the unique capabilities of the next generation neutron multiplicity detector–Multiplicity Counter-15 (MC-15)–to time-tag and bin the data into time-correlation histograms. This algorithm is more robust than other algorithms that only rely on the neutron count rate because it is able to identify the presence of neutron chains from highly enriched uranium, which has a small neutron emission rate. The presence of neutron chains is unique to special nuclear material (SNM) and can be used to differentiate between threat-quantities of SNM and industrial sources. This algorithm will be demonstrated on a computer connected to an MC-15 and will utilize the time-correlation histograms that are created in real-time on-board the MC-15. The graphical user interface will update the status of the threat-identification in real-time as more data is collected. This algorithm will be implementable onto the MC-15, which is deployed to multiple emergency response teams. The inclusion of this algorithm onto the MC-15 will expedite which courses of action can be taken and will increase the efficiency of these teams in mitigating these problems.

Technical Outcomes

The method explored ratios of the single, double, and triple neutron correlation rates and looked for clustering. Over seven thousand previously acquired measurements of items containing plutonium (Pu), uranium (U), californium (Cf), industrial-type sources and non-radiological material were evaluated. The ratios that were calculated from these measurements were plotted and collated by material type to identify trends. In general there was good separation between special nuclear material (SNM), and non-SNM sources. In some cases, however, overlap exists that requires additional investigation.

From 1-Dimensional Sequence to 3-Dimensional Genomes: An Exascale Human Genome Project for the Next Generation of Biological Inquiry

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Project Description

Los Alamos scientists initiated the first Human Genome Project, resulting in the complete mapping of the one dimensional (1-D) structure (sequence) of a human genome. However, 30+ plus years later, new scientific evidence indicates that these 1-D maps have limitations. We now know that the same genome sequence can have dramatically different three dimensional structures and chemical modifications (epigenetic marks) that alter the function of the deoxyribonucleic acid (DNA). Thus, to more accurately characterize an organism's genome, 3-D structures need to be determined for as many cell types and environments as possible. This project will conduct research that will lay the groundwork for establishing new methods (and standards) to model, visualize, and interact with the 3D architecture of an organism's genome across different scales of resolution. This work will have profound implications for host-pathogen interactions (biothreat), bioenergy, and foundational biological inquiry. Once developed, this technology will directly support energy security initiatives (renewable energy), further understanding of climate and energy Impacts on biological systems, and will contribute to national defense strategies for pathogen detection and countermeasures.

Technical Outcomes

This project used simulations to make 3-Dimensional models of chromosomes and visualized the models. The models agreed with experimental data, providing confidence in the models. The team could see the intricate shapes and structures of the chromosome and pinpoint the location of critical genes. The team evaluated existing technology for chromosome visualization and made plans for new, more useful 3D viewers that use these techniques.

Publications

Reports

Hovde, B., W. L. K. M. Eng and S. R. Starkenburg. Summer 2020 Internship Report. Unpublished report. (LA-UR-20-26946)

Modeling Hospital/Healthcare Surge Capacity in Response to Coronavirus (COVID-19)

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Project Description

The current Coronavirus Disease 2019 (COVID-19) pandemic poses a considerable national and international public health challenge as well as national security challenge due to the economic and population impacts. Thus, assessing the potential impacts of COVID-19 on the healthcare and public healthcare sector can help us prepare and respond to this national and global emergency. This project will address this challenge by extending the Disease Infection National Forecast for Evolving Contagion Trends (DISINFECT) model to include hospitals and resources (e.g., regular beds, intensive care unit beds, and testing kits) to assess magnitude, extent, and duration of impacts on the healthcare system at various spatial scales and by age/comorbidity risk factors.

Technical Outcomes

This project was instrumental in helping develop weekly hospitalization forecasts for the U.S. at the state-level in support of the Centers for Disease Control and Prevention (CDC) Coronavirus forecast hospitalization effort as well as in supporting the New Mexico Department of Health by providing regional hospitalization forecasts to inform resource allocation. In addition, the team analyzed patient data and assessed the impact of co-morbidities, demographics, movement, and resource utilization in predicting negative health outcomes.

Publications

Journal Articles

Castro, L. A., C. D. Shelley, D. A. Osthus, I. J. Michaud, J. Mitchell, C. A. Manore and S. Y. Del Valle. How New Mexico Leveraged a COVID-19 Case Forecasting Model to Preemptively Address the Healthcare Needs of the State: A Quantitative Analysis. Submitted to *JMIR Public Health and Surveillance*. (LA-UR-21-21597)

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. Submitted to *Health Policy OPEN*. (LA-UR-20-30424)

Picard, R. R. and D. A. Osthus. Forecast Intervals for Infectious Disease Models. Submitted to *International Journal of Forecasting*. (LA-UR-20-29644)

Shelley, C. D., G. Rajasekar, M. K. Lieng and M. Nu\xc3\xb1o. Characteristics and Severity of COVID-19 Patients in Five Academic Hospitals in California. Submitted to *Journal of Epidemiology & Community Health*. (LA-UR-21-20303)

Presentation Slides

Castro, L. A. and C. D. Shelley. Leveraging a COVID-19 Case Forecasting Model for Predicting Health Care Needs in New Mexico: A Quantitative Analysis. . (LA-UR-21-20636)

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)

Manore, C. A., C. D. Shelley and S. Y. Del Valle. Mathematical Modeling of COVID-19: Understanding the Impact of School Reopening. Presented at *Kiwanis*, Los Alamos, New Mexico, United States, 2020-07-07 - 2020-07-07. (LA-UR-20-24955)

Del Valle, S. Y. Real-time Data Fusion to Guide Disease Forecasting Models. Presented at *SIAM Conference on Life Sciences*, Los Alamos, New Mexico, United States, 2020-06-18 - 2020-06-18. (LA-UR-20-24388)

Del Valle, S. Y. Real-time Data Fusion to Guide Forecasting Models. . (LA-CP-20-20508)

Del Valle, S. Y., P. S. Chadwick, C. D. Shelley and C. A. Manore. COVID-19 School Reopening Schedule Research. . (LA-UR-20-25499)

Del Valle, S. Y. and D. A. Osthus. Epidemic Modeling Capabilities at Los Alamos National Laboratory. . (LA-UR-20-23969)

Misinformation and Critical Disease Transmission Behaviors in Online Data

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Project Description

Misinformation around the current SARS-CoV-2 (the virus that causes COVID-19) outbreak has potentially deadly consequences. One report shows examples of incorrect information about fake cures or treatments, fake testing kits, and conspiracy theories about the origin of the virus. Misinformation can cause individuals to act in ways that increase the spread of the disease, risking the health of others that may be more prone to complications from the disease. We use social media and internet data, and supervised and unsupervised machine learning algorithms to understand (1) the types of misinformation and their spread and (2) human behaviors that contribute to the transmission of COVID-19. This work will be used to understand the impacts of misinformation in infectious diseases, and will be used to inform other modeling (e.g., forecasting) efforts at LANL.

Technical Outcomes

This project used supervised and unsupervised machine learning algorithms to understand themes in misinformation, misinformation spread, and public health-relevant human behaviors in social media and internet data. The team explored a dozen common myths, provided a detailed exploration of four conspiracy theories in Twitter and in Reddit, labeled over 7,000 tweets for behaviors related to Coronavirus (COVID-19), built natural language processing algorithms to identify specific relevant behaviors, and provided analysis of trends in these behaviors.

Publications

Journal Articles

Daughton, A. R., C. D. Shelley, M. J. Barnard, D. J. Gerts, C. M. Watson Ross, I. K. Crooker, G. S. Nadiga, N. Mukundan, T. R. Pitts, N. Y. Vaquera Chavez and G. Fairchild. Mining social media for COVID-19 related Human Behaviors. Submitted to *Journal of Medical Internet Research*. (LA-UR-21-20074)

Gerts, D. J., C. D. Shelley, N. K. Parikh, T. R. Pitts, C. M. Watson Ross, G. Fairchild, N. Y. Vaquera Chavez and A. R. Daughton. “Thought I’d Share First”: An Analysis of COVID-19 Conspiracy Theories and Misinformation Spread on Twitter. Submitted to *Journal of Medical Internet Research*. (LA-UR-20-28305)

Presentation Slides

Daughton, A. R., T. R. Pitts, C. M. Watson Ross, C. D. Shelley, G. Fairchild, N. K. Parikh, D. J. Gerts and N. Y. Vaquera Chavez. Mining Social Media for COVID-19 Information. Presented at *DOE Summit*, Virtual, New Mexico, United States, 2020-07-14 - 2020-07-15. (LA-UR-20-24909)

Mccabe, K. J. COVID-19 Modeling for Pandemic Response. . (LA-UR-20-28906)

Mccabe, K. J. COVID-19 Modeling for Pandemic Response. . (LA-UR-20-29022)

Mccabe, K. J. and R. E. McDonald. Global Disease Modeling & Forecasting Center. . (LA-UR-20-27812)

Lifeline: an Extensible, Agent-Based Model for Critical Healthcare Supply Chains

Nidhi Parikh
20200733ER

Project Description

The coronavirus (COVID-19) pandemic is an unprecedented national security challenge, with the nation's public health system at the front lines of the battle to control the outbreak. The system depends utterly on its ability to acquire necessary equipment and supplies, ranging from simple masks and gowns to sophisticated medical devices like ventilators. The goal of this project is to allow planners at the state and federal level to make effective and timely decisions on the acquisition, allocation, and distribution of medical resources, by producing a supply-chain model that can readily adapt to rapidly changing circumstances. Together with ongoing epidemic and hospital demand modeling efforts, the supply-chain model will track critical supplies from any number of sources to the hospitals and clinics that will consume them using best available data in real-time. We intend to produce a working model within a few weeks, capable of informing decision makers at the state and regional level, and will extend it to national scale in four to five months, in time to prepare for seasonal resurgence of the pandemic in the fall.

Technical Outcomes

This project created the missing computational tool needed to plan optimal healthcare supplies production, stockpile, and distribution scheduling (i.e., the supply chain). The team developed an agent-based model of healthcare supply chain (Lifeline) that provides decision makers with the capability to manage health care supplies in time and space so as to avoid catastrophic impacts from the current coronavirus pandemic, as well as from similar healthcare emergencies in the future.

Numerical Methods for Radiation Hydrodynamics Simulations on Current and Future Advanced Parallel Architectures

Jonas Lippuner
20190519ECR

Project Description

To ensure the safety and reliability of the United States nuclear stockpile, large-scale, sophisticated, multi-physics computer simulations of nuclear explosions are necessary since the US does not conduct nuclear tests anymore. To perform these simulations, the Department of Energy operates the largest supercomputers in the world. The computing hardware in these supercomputers has changed dramatically in the last decade and most of the computing power (up to 95%) is now in special, advanced architecture chips, such as graphics processing units (GPUs). The simulation codes used today were designed long before these chips were invented and the methods and algorithms used in our codes are not necessarily the best suited ones for the current and future hardware. This project seeks to investigate which methods perform most efficiently on this advanced hardware and to develop new such methods. The results of this work will be crucial to decide the future direction of the various programmatic simulation code development efforts of the National Nuclear Security Administration. The new methods developed as part of this project will also help ensure that our large-scale physics simulations run efficiently on current and future supercomputers.

Publications

Journal Articles

Fernandez, R., F. Foucart and J. Lippuner. The landscape of disk outflows from black hole - neutron star mergers. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-23877)

Lippuner, J. Ethon: A software framework for hydrodynamics simulations with block-based AMR on parallel computing architectures. Submitted to *SoftwareX*. (LA-UR-21-20255)

Reports

Lippuner, J. Ethon hydrodynamics notes. Unpublished report. (LA-UR-20-30347)

Improving Predictions of Complex Systems with Predictive Discrepancy Models and Data Fusion

David Osthus
20190546ECR

Project Description

Disease spread represents a vulnerability and risk to our national security. Pandemics don't respect borders and pose a significant burden on our populace and infrastructure. Intervention strategies are only successful if deployed in a timely, efficient, and targeted manner. Preferably, interventions are proactive rather than reactive. Before we can proactively counter disease spread, however, we have to be able to forecast its spread. Thus, disease forecasting capabilities constitute a significant link in the national security chain. This project will develop state, regional, and national flu forecasting models that will be deployed in real-time to maximize impact with public health decision makers. These models will push the limits of disease forecasting by bringing together state-of-the-art mathematical modeling with numerous data sources. The mathematical modeling advances are relevant to many applications with incomplete theory, experimental data, and the need to make predictions with quantified uncertainties. As such, this work has broad applicability to Department of Energy and National Nuclear Security Administration applications, such as nuclear weapons, nonproliferation, and energy, as well as direct applications in National Institutes of Health and Centers for Disease Control and Prevention.

Publications

Journal Articles

Gibson, G. C., D. A. Osthus, K. R. Moran and N. G. Reich. Improving Probabilistic Infectious Disease Forecasting Through Coherence. Submitted to *PLOS Computational Biology*. (LA-UR-19-32598)

Osthus, D. A. Fast and Accurate Influenza Forecasting in the United States with Inferno. Submitted to *PLOS Computational Biology*. (LA-UR-20-30384)

Osthus, D. A. and K. R. Moran. Multiscale influenza forecasting. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-19-28977)

Picard, R. R. and D. A. Osthus. Forecast Intervals for Infectious Disease Models. Submitted to *International Journal of Forecasting*. (LA-UR-20-29644)

Shelley, C. D., G. Rajasekar, M. K. Lieng and M. Nu\xc3\xb1o. Characteristics and Severity of COVID-19 Patients in Five Academic Hospitals in California. Submitted to *Journal of Epidemiology & Community Health*. (LA-UR-21-20303)

Presentation Slides

Castro, L. A. The evolution of COVID-19 forecasting: What went right, what went wrong, and how do we do better next time. . (LA-UR-21-20686)

Castro, L. A. and C. D. Shelley. Leveraging a COVID-19 Case Forecasting Model for Predicting Health Care Needs in New Mexico: A Quantitative Analysis. . (LA-UR-21-20636)

Osthus, D. A. Dante: An Applied Statistician's Approach to Flu Forecasting. Presented at *FluSight Seasonal Influenza Forecasting Workshop*, Atlanta, Georgia, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28213)

Osthus, D. A. Dante: An Applied Statistician's Approach to Flu Forecasting. . (LA-UR-19-28798)

Osthus, D. A. What we've learned from 7 years of real-time flu forecasting in the United States. Presented at *Joint Statistical Meetings*, Online, New Mexico, United States, 2020-08-02 - 2020-08-02. (LA-UR-20-25785)

Osthus, D. A. and K. R. Moran. Multiscale Flu Forecasting. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-28 - 2019-07-28. (LA-UR-19-27237)

Posters

Osthus, D. A. 2018/19 FluSight Challenge Dante and DBM +. Presented at *FluSight Seasonal Influenza Forecasting Workshop*, Atlanta, Georgia, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28198)

Optimizing Scientific Codes in the Presence of Extreme Heterogeneity Using Machine Learning

Eun Jung Park
20190566ECR

Project Description

Existing hint-based approaches to optimizing the translation of human code to machine code for complex scientific codes have been effective at generating efficient code for traditional architectures, but emerging heterogeneous architectures have proven too complex for existing techniques. This project will leverage emerging machine learning techniques to perform code translation for complex, heterogeneous machine architectures. The resulting techniques will be one critical step in supporting scientific computing on the non-traditional computer architectures expected to replace existing supercomputing platforms in the post-Exascale era.

Discrete Optimization Algorithms for Provably Optimal Quantum Circuit Design

Harsha Nagarajan

20190590ECR

Project Description

As stated in the 2018 United States national strategic overview for Quantum Information Science (QIS), "QIS applies the best understanding of the sub-atomic world—quantum theory—to generate new knowledge and technologies. Prior applications of QIS-related technologies include semiconductor microelectronics, the global positioning system (GPS), and magnetic resonance imaging (MRI). These also underpin significant parts of the national economic and defense infrastructure". QIS, applied in quantum computers, has the potential to dramatically outperform classical computers. Research and development in QIS is one of the the Department of Energy's growth areas. This project is focused squarely on building the fundamental algorithms that reduce the computational burden and provide new design architectures that facilitate the ability of DOE policy makers to make informed decisions on the design of next-generation quantum computers. The algorithms developed in this project will have a direct impact on the Laboratory's research missions. Also, due to the fundamental nature of this project, it will build underlying capability with likely future applicability to DOE Office of Electricity (OE) needs such as the "Networked Microgrids" and "Resilient Design Tool for Distribution Networks" projects.

Publications

Journal Articles

Bhela, S., H. Nagarajan, D. Deka and V. Kekatos. Efficient Topology Design Algorithms for Power Grid Stability. Submitted to *IEEE Control Systems Letters*. (LA-UR-21-22364)

Ryu, M., H. Nagarajan and R. W. Bent. Mitigating the Impacts of Uncertain Geomagnetic Disturbances on Electric Grids: A Distributionally Robust Optimization Approach. Submitted to *IEEE Transactions on Power Systems*. (LA-UR-21-22568)

Automatic Colormap Improvement in non-Euclidean Spaces

Roxana Bujack
20200512ECR

Project Description

The work suggested in this proposal 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.

Publications

Conference Papers

Nardini, P. A., M. Chen, M. Boettinger, G. Scheuermann and R. B. Bujack. Automatic Improvement of Continuous Colormaps in Euclidean Colorspaces. Presented at *IEEE Vis*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-19-29080)

Nardini, P. A., M. Chen, R. B. Bujack 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)

Other

Bujack, R. B. Geodesics in Color Space. Dataset. (LA-UR-21-22239)

Enhancing Bayesian Multivariate Adaptive Regression Spline Models Using Concepts from Deep Learning

Devin Francom
20200571ECR

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.

Publications

Journal Articles

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)

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

Shen, A. A., D. C. Francom and K. N. Rumsey. Robust Bayesian Multivariate Adaptive Regression Splines (BMARS). . (LA-UR-20-27874)

Differentiable Programming: Bridging the Gap between Numerical Models and Machine Learning Models

Daniel O'Malley
20200575ECR

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).

Publications

Journal Articles

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. Submitted to *Expert Systems with Applications*. (LA-UR-21-20260)

Presentation Slides

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)

Distributed Algorithms for Large-Scale Ordinary Differential/Partial Differential Equation (ODE/PDE) Constrained Optimization Problems on Graphs

Kaarthik Sundar
20200603ECR

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.

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 *IEEE Transactions on Robotics*. (LA-UR-21-20249)

Sundar, K., S. Sanjeevi and H. Nagarajan. Sequence of Polyhedral Relaxations for Nonlinear Univariate Functions. Submitted to *Optimization and Engineering*. (LA-UR-20-23980)

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)

Advancing Discrete Fracture Matrix Models using Topologically Driven System Reduction

Jeffrey Hyman
20180579ECR

Project Description

The model resulting from this project will allow Laboratory researchers to probe fundamental science questions concerning subsurface transport in fractured media. It is of interest to the Department of Energy's Offices of Fossil Energy and Energy Efficiency & Renewable Energy (EERE) programs as well as the DOE initiatives Subsurface Technology and Engineering Research (SubTER) and Energy-Water Nexus. In particular, the model will help predict how much hydrocarbon remains in unconventional reservoirs after production has ceased (by some estimates up to 70% is left behind), accurate calculations of when trace chemicals from an underground explosion will reach the surface, and promote successful environmental management strategies. This project also supports mission pillars of energy security (subsurface hydrocarbon acquisition, geothermal energy extraction, carbon sequestration), global security (Defense Threat Reduction Agency gas migration from underground low yield nuclear weapons testing), and stockpile stewardship (brittle material failure prediction).

Technical Outcomes

The project developed a high-fidelity three-dimensional discrete fracture matrix model to simulate flow and transport in fractured subsurface media. The model combines a graph-theory based approach to partition the network into two disjoint subnetworks with a novel algorithm to mesh the rock matrix around the fracture network. Once this is complete, the team discretizes the governing equations for flow and transport in the fractures and matrix using mimetic finite difference methods and couple the two systems.

Publications

Journal Articles

*Berrone, S., J. D. Hyman and S. Pieraccini. Multilevel Monte Carlo Predictions of First Passage Times in Three-Dimensional Discrete Fracture Networks: A Graph-Based Approach. 2020. *Water Resources Research*. **56** (6): e2019WR026493. (LA-UR-19-29755 DOI: 10.1029/2019WR026493)

Doolaeghe, D., J. D. Hyman, P. Davy and C. Darcel. A Graph-based flow modeling approach adapted to multiscale Discrete Fracture Network models. Submitted to *Physical Review E*. (LA-UR-20-25066)

Hyman, J. D. Flow Channeling in Fracture Networks: Characterizing the Effect of Fracture Density on Preferential Flow Path Formation. Submitted to *Water Resources Research*. (LA-UR-20-23557)

Hyman, J. D., H. M. Ushijima-Mwesigwa, A. A. Hagberg, I. Safro, S. Karra, C. W. Gable and G. Srinivasan. Multilevel Graph Partitioning for Three-Dimensional Discrete Fracture Network Flow Simulations. Submitted to *SIAM Journal on Scientific Computing*. (LA-UR-19-21113)

*Hyman, J. D., H. Rajaram, S. Srinivasan, N. Makedonska, S. Karra, H. Viswanathan and G. Srinivasan. Matrix Diffusion in Fractured Media: New Insights Into Power Law Scaling of Breakthrough Curves. 2019. *Geophysical Research Letters*. **46** (23): 13785-13795. (LA-UR-19-23625 DOI: 10.1029/2019GL085454)

*Hyman, J. D., J. Jimenez-Martinez, C. W. Gable, P. H. Stauffer and R. J. Pawar. Characterizing the Impact of Fractured Caprock Heterogeneity on Supercritical CO_2 Injection. 2020. *Transport in Porous Media*. **131** (3): 935-955. (LA-UR-19-25316 DOI: 10.1007/s11242-019-01372-1)

Hyman, J. D., M. Dentz, A. A. Hagberg and P. Kang. What Controls Asymptotic Transport Properties in Fractured Media? Uncovering a Connection Between Fracture Network Properties and Particle Behavior. Submitted to *Geophysical Research Letters*. (LA-UR-18-29270)

*Hyman, J. D., M. Dentz, A. Hagberg and P. K. Kang. Linking Structural and Transport Properties in Three-Dimensional Fracture Networks. 2019. *Journal of Geophysical Research: Solid Earth*. **124** (2): 1185-1204. (LA-UR-18-27717 DOI: 10.1029/2018JB016553)

*Hyman, J. D., M. Dentz, A. Hagberg and P. K. Kang. Emergence of Stable Laws for First Passage Times in Three-

Dimensional Random Fracture Networks. 2019. *Physical Review Letters*. **123** (24): 248501. (LA-UR-19-23405 DOI: 10.1103/PhysRevLett.123.248501)

Kang, P. K., J. D. Hyman, W. S. Han and M. Dentz. Anomalous Transport in Three-Dimensional Discrete Fracture Networks: Interplay between Aperture Heterogeneity and Particle Injection Modes. Submitted to *Physical Review Fluids*. (LA-UR-20-20512)

Osthus, D. A., J. D. Hyman, S. Karra, N. Panda and G. Srinivasan. A Probabilistic Clustering Approach for Identifying Primary Subnetworks of Discrete Fracture Networks with Quantified Uncertainty. Submitted to *SIAM/ASA Journal on Uncertainty Quantification*. (LA-UR-19-27288)

*Romano, V., S. Bigi, F. Carnevale, J. De'Haven Hyman, S. Karra, A. J. Valocchi, M. C. Tartarello and M. Battaglia. Hydraulic characterization of a fault zone from fracture distribution. 2020. *Journal of Structural Geology*. **135**: 104036. (LA-UR-19-32302 DOI: 10.1016/j.jsg.2020.104036)

Sherman, T., G. Sole-Mari, J. D. Hyman, M. R. Sweeney, D. Vassallo and D. Bolster. Characterizing Reactive Transport Behavior in a Three Dimensional Discrete Fracture Network. Submitted to *Transport in Porous Media*. (LA-UR-20-26548)

*Sherman, T., J. D. Hyman, D. Bolster, N. Makedonska and G. Srinivasan. Characterizing the impact of particle behavior at fracture intersections in three-dimensional discrete fracture networks. 2019. *Physical Review E*. **99** (1): 013110. (LA-UR-18-29382 DOI: 10.1103/PhysRevE.99.013110)

*Sherman, T., J. Hyman, M. Dentz and D. Bolster. Characterizing the Influence of Fracture Density on Network Scale Transport. 2020. *Journal of Geophysical Research: Solid Earth*. **125** (1). (LA-UR-19-27671 DOI: 10.1029/2019JB018547)

Srinivasan, S., D. O'Malley, J. D. Hyman, S. Karra, H. S. Viswanathan and G. Srinivasan. Transient flow modeling in fractured media using graphs. Submitted to *Physical Review E*. (LA-UR-20-23560)

Srinivasan, S., E. Cawi, J. D. Hyman, D. A. Osthus, A. A. Hagberg, H. S. Viswanathan and G. Srinivasan. Physics-Informed Machine Learning for Backbone Identification in Discrete Fracture Networks. Submitted to *Computational Geosciences*. (LA-UR-19-28357)

Sweeney, M. R., C. W. Gable, S. Karra, P. H. Stauffer, R. J. Pawar and J. D. Hyman. Upscaled discrete fracture matrix model (UDFM): an octree-refined continuum representation of fractured porous media. Submitted to *Computational Geosciences*. (LA-UR-19-25805)

Sweeney, M. R. and J. D. Hyman. Stress effects on flow and transport in three-dimensional fracture networks. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-19-30234)

Presentation Slides

Hyman, J. D. Applications of Graph Theory and Machine Learning to Discrete Fracture Networks. . (LA-UR-18-31148)

Hyman, J. D. The Influence of Multiple Scales in Fractured Media on Flow and Transport Properties. . (LA-UR-18-30105)

Hyman, J. D. FRAM. Presented at *dfnWorkShop*, SANTA FE, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29484)

Hyman, J. D. pydfnworks. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29482)

Hyman, J. D. background slides for dfnWorkShop. Presented at *dfnworkshop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29494)

Hyman, J. D. Flow Channeling in Fracture Networks. Presented at *SKB workshop*, Online, New Mexico, United States, 2020-10-20 - 2020-10-20. (LA-UR-20-28373)

Hyman, J. D., H. Rajaram, S. Srinivasan, N. Makedonska, S. Karra, H. S. Viswanathan and G. Srinivasan. The role of advection and matrix diffusion in power-law scaling behavior of first passage times in three-dimensional discrete fracture networks. Presented at *AGU fall Meeting*, San Fransisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-31973)

Hyman, J. D., J. Jimenez-Martinez and R. J. Pawar. Characterizing the Impact of Fracture Geometry and Network Structure on Multiphase Flow through Fractured Media. Presented at *AGU Fall Meeting*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31334)

Sweeney, M. R. Modeling discrete fracture networks in porous media using a continuum approach. Presented at *Arizona - Los Alamos Days*, Tucson, Arizona, United States, 2019-04-20 - 2019-04-21. (LA-UR-19-23513)

Sweeney, M. R. Leveraging the dfnWorks software suite for continuum modeling of fractured porous media. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29299)

Sweeney, M. R., J. D. Hyman, C. W. Gable, S. Karra, N. Makedonska and R. J. Pawar. Octree-refined continuum representation of discrete fracture networks. Presented at *SIAM Geoscience 2019*, Houston, Texas, United States, 2019-03-11 - 2019-03-11. (LA-UR-19-22018)

Posters

Kang, P., J. D. Hyman and M. Dentz. Anomalous Transport in 3D Discrete Fracture Networks (DFN): Interplay between Aperture Heterogeneity and Particle Injection Modes. Presented at *AGU Fall Meeting*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31476)

Sherman, T. J., D. Bolster, N. Makedonska, G. Srinivasan and J. D. Hyman. Characterizing the impact of Lagrangian particle behavior at fracture intersections on transport through three-dimensional fracture networks. Presented at *American Geophysical Union Fall 2018*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31288)

Sweeney, M. R. and J. D. Hyman. How do different stress regimes affect transport in three-dimensional discrete fracture networks?. Presented at *LANL Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28466)

Sweeney, M. R. and J. D. Hyman. How do different stress networks affect transport in three-dimensional discrete fracture networks?. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29295)

Robust Anomaly Detection in Complex Networks: Data Fusion and New-Link Prediction

Melissa Turcotte
20180607ECR

Project Description

Cybersecurity is one of the most important challenges that the U.S. Government currently faces, as indicated by Presidential Policy Directive 20 and the Comprehensive National Cybersecurity Initiative. Detection of cyber-attacks traditionally relies heavily on rule-based (or signature-based) intrusion detection systems, which are powerful tools but require specific threat signatures previously observed from attacks. As a result, they are fragile and are easily subverted by attacks with previously unknown or unidentified signatures. In contrast, anomaly detection systems offer an orthogonal defense; by dynamically learning models of normal behavior and detecting deviations to identify new variants of attacks. In spite of more than two decades of research on anomaly detection for cyber defense, operational use is still nascent primarily because of high false positive rates and un-interpretable alerts. This work aims to tackle these two problems by developing models for new links (previously unobserved relationships between network entities) in relational network data thereby reducing false alarms to practical levels and building causal relationship graphs of malicious behavior by combining "weak" signals crossing multiple cyber data sets both reducing false alarms and providing key event context enhancing the usefulness of anomaly detection in operational cyber defense.

Technical Outcomes

Extensions to a Poisson matrix factorisation (PMF) model were developed to improve graph link prediction. The extensions includes scenarios that are commonly encountered in cyber and national security applications yet not accounted for in existing models. The use of generative hyper-heuristic search algorithms to automate the selection and generation of customized link prediction algorithms according to the specific problem and data set were also developed.

Publications

Journal Articles

Turcotte, M., F. Sanna Passino and N. A. Heard. GRAPH LINK PREDICTION IN COMPUTER NETWORKS USING POISSON MATRIX FACTORISATION. Submitted to *Annals of Applied Statistics*. (LA-UR-20-20567)

Turcotte, M., K. L. Hallgren and N. A. Heard. Changepoint detection on a graph of time series. Submitted to *Bayesian Analysis*. (LA-UR-21-22411)

Conference Papers

Pope, A. S., D. R. Tauritz and M. Turcotte. Automated Design of Tailored Link Prediction Heuristics for Applications in Enterprise Network Security. Presented at *The Genetic and Evolutionary Computation Conference*. (Prague, Czech Republic, 2019-07-13 - 2019-07-17). (LA-UR-19-23176)

Reports

Pope, A. S. The Automated Design of Network Graph Algorithms with Applications in Cybersecurity. Unpublished report. (LA-UR-20-20273)

Presentation Slides

Y. Hallgren, K. L. and M. Turcotte. Robust Bayesian change detection for cyber-security applications. . (LA-UR-20-20324)

Sanna Passino, F., M. Turcotte and N. Heard. Some ideas on Bayesian modelling of networks for cyber-security applications. Presented at *Focused Research Workshop*, Bristol, United Kingdom, 2019-03-25 - 2019-03-28. (LA-UR-19-23198)

Turcotte, M. Latent Feature Models for Network Link Prediction with Labelled Nodes. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-27 - 2019-07-27. (LA-UR-19-27254)

Posters

Sanna Passino, F. and M. Turcotte. Latent feature models for network link prediction with labelled nodes. . (LA-UR-18-26824)

Other

Turcotte, M. Unified Host and Network Dataset - Supplement. Dataset. (LA-UR-18-27853)

Machine Learning of Quantum Computing Algorithms

Patrick Coles
20180628ECR

Project Description

Building a quantum computer has been compared to the Manhattan Project, in that achieving the goal will have widespread effects, even at the geo-political level. Quantum computers promise to revolutionize various fields like pharmaceutical design and big-data analysis. A quantum computer would impact both financial and national security, since it could be used to break our current methods for encrypted communication. Furthermore, our national nuclear security could benefit from quantum computers, since they may speed up our ability to optimize weapons design and to simulate explosion dynamics. However, none of these impacts will be realized without well-designed algorithms. In other words, exploiting recent advances in quantum computing hardware (e.g., made by US companies like Google, IBM, and Intel) will require efficient software. Our work will address this software issue by automating the process of designing quantum computing algorithms. Our software will determine the fastest algorithm for a specific hardware and a specific application. For example, suppose one wants to use a quantum computer to simulate a biological molecule. Our software will find the fastest algorithm for this – taking into account the imperfections of the hardware. This will be a crucial tool for using real quantum computers in the future.

Technical Outcomes

The project developed a framework (and software code) for automating the process of quantum algorithm design based on machine learning. The research extended this framework to account for imperfections in the hardware. The project made this framework scalable using quantum machine learning (QML). The project invented QML algorithms for various applications including linear systems, dynamical simulation, and data analysis. The researchers developed tools to analyze the scalability of QML.

Publications

Journal Articles

Arrasmith, A. T., L. Cincio, R. D. Somma and P. J. Coles. Operator Sampling for Shot-frugal Optimization in Variational Algorithms. Submitted to *npj Quantum Information*. (LA-UR-20-22810)

Arrasmith, A. T., P. J. Czarnik, P. J. Coles and L. Cincio. Error Mitigation with Clifford quantum-circuit data. Submitted to *Physical Review Letters*. (LA-UR-20-23755)

Bilkis, M., M. V. S. Cerezo de la Roca, G. Verdon, P. J. Coles and L. Cincio. A semi-agnostic ansatz with variable structure for quantum machine learning. Submitted to *Quantum*. (LA-UR-21-22040)

Bravo-Prieto, C., R. LaRose, M. V. S. Cerezo de la Roca, Y. Subasi, L. Cincio and P. J. Coles. Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems. Submitted to *arXiv*. (LA-UR-19-29101)

Cerezo, M., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation. 2020. *Quantum*. **4**: 248. (LA-UR-19-25585 DOI: 10.22331/q-2020-03-26-248)

Cincio, L., K. Rudinger, M. Sarovar and P. J. Coles. Machine learning of noise-resilient quantum circuits. Submitted to *PRX, arxiv*. (LA-UR-20-24253)

*Coles, P. J., M. Cerezo and L. Cincio. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states. 2019. *Physical Review A*. **100** (2): 022103. (LA-UR-19-22724 DOI: 10.1103/PhysRevA.100.022103)

Holmes, Z. P., K. Sharma, M. V. S. Cerezo de la Roca and P. J. Coles. Connecting ansatz expressibility to cost gradients and barren plateau. Submitted to *Quantum*. (LA-UR-21-20034)

Khatri, S., R. LaRose, A. Poremba, L. Cincio, A. T. Sornborger and P. J. Coles. Quantum-assisted quantum compiling. 2019. *Quantum*. **3**: 140. (LA-UR-18-25861 DOI: 10.22331/q-2019-05-13-140)

*Kuebler, J. M., A. Arrasmith, L. Cincio and P. J. Coles. An Adaptive Optimizer for Measurement-Frugal Variational Algorithms. 2020. *Quantum*. **4**: 263. (LA-UR-19-29383 DOI: 10.22331/q-2020-05-11-263)

*LaRose, R., A. Tikku, E. O'Neel-Judy, L. Cincio and P. J. Coles. Variational quantum state diagonalization. 2019. *npj*

Quantum Information. **5** (1): 57. (LA-UR-18-29266 DOI: 10.1038/s41534-019-0167-6)

S. Cerezo de la Roca, M. V., A. Sone, J. Beckey and P. J. Coles. A Generalized Measure of Quantum Fisher Information. Submitted to *Physical Review A*. (LA-UR-20-27870)

S. Cerezo de la Roca, M. V., A. Sone, T. J. Volkoff, L. Cincio and P. J. Coles. Cost-Function-Dependent Barren Plateaus in Shallow Quantum Neural Networks. Submitted to *Nature Communications*. (LA-UR-19-32681)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio and P. J. Coles. Variational Quantum Algorithms. Submitted to *Nature Reviews Physics*. (LA-UR-20-30142)

S. Cerezo de la Roca, M. V., K. Sharma, A. T. Arrasmith and P. J. Coles. Variational Quantum State Eigensolver. Submitted to *Nature Partner Journal Quantum Information*. (LA-UR-20-22660)

S. Cerezo de la Roca, M. V. and P. J. Coles. Impact of Barren Plateaus on the Hessian and Higher Order Derivatives. Submitted to *Physical Review A*. (LA-UR-20-26309)

Sharma, K., M. V. S. Cerezo de la Roca, L. Cincio and P. J. Coles. Trainability of Dissipative Perceptron-Based Quantum Neural Networks. Submitted to *Physical Review Letters*. (LA-UR-20-23484)

Sharma, K., M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio, A. T. Sornborger and P. J. Coles. Reformulation of the No-Free-Lunch Theorem for Entangled Data Sets. Submitted to *Nature Physics*. (LA-UR-20-25010)

*Sharma, K., S. Khatri, M. Cerezo and P. J. Coles. Noise resilience of variational quantum compiling. 2020. *New Journal of Physics*. **22** (4): 043006. (LA-UR-19-28095 DOI: 10.1088/1367-2630/ab784c)

Sornborger, A. T., B. A. Commeau, M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio and P. J. Coles. \xef\xbb\xbfVariational Hamiltonian Diagonalization for Dynamical Quantum Simulation. Submitted to *Quantum*. (LA-UR-20-26827)

*Subasi, Y., L. Cincio and P. J. Coles. Entanglement spectroscopy with a depth-two quantum circuit. 2019. *Journal of Physics A: Mathematical and Theoretical*. **52** (4): 44001. (LA-UR-18-25483 DOI: 10.1088/1751-8121/aaf54d)

*Di Tullio, M., R. Rossignoli, M. Cerezo and N. Gigena. Fermionic entanglement in the Lipkin model. 2019. *Physical Review A*. **100** (6): 062104. (LA-UR-19-27998 DOI: 10.1103/PhysRevA.100.062104)

Volkoff, T. J. and P. J. Coles. Large gradients via correlation in random parameterized quantum circuits. 2021. *Quantum Science and Technology*. **6** (2): 25008. (LA-UR-20-23818 DOI: 10.1088/2058-9565/abd891)

Zhang, Y., P. J. Coles, A. Winick, J. Lin and N. Lutkenhaus. Security proof of practical quantum key distribution with detection-efficiency mismatch. Submitted to *Physical Review A*. (LA-UR-20-22369)

Reports

S. Cerezo de la Roca, M. V. and P. J. Coles. Comment on "Characterizing the loss landscape of variational quantum circuits". Unpublished report. (LA-UR-20-26075)

Presentation Slides

Arrasmith, A. T., J. Kubler, L. Cincio, R. D. Somma and P. J. Coles. Shot Frugal Optimization for VQE. Presented at *Quantum Techniques in Machine Learning 2020*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-29153)

Coles, P. J. Quantum computing in the NISQ era. Presented at *quantum computing summer school*, Los Alamos, New Mexico, United States, 2020-06-09 - 2020-06-09. (LA-UR-20-24251)

S. Cerezo de la Roca, M. V. Talk: Trainability of Quantum Neural Network. . (LA-UR-20-24280)

S. Cerezo de la Roca, M. V. Science in 3. . (LA-UR-20-25832)

S. Cerezo de la Roca, M. V. Talk: Variational Quantum State Eigensolver. Presented at *QuAlg*, virtual, New Mexico, United States, 2020-09-22 - 2020-09-22. (LA-UR-20-27347)

Posters

S. Cerezo de la Roca, M. V., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation (VQFE). . (LA-UR-19-28193)

S. Cerezo de la Roca, M. V., L. Cincio and P. J. Coles. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states Or, how to compare two quantum states on a quantum computer. . (LA-UR-19-24875)

Emergent Quantum Phenomena with Tensor Networks

Lukasz Cincio
20190659PRD4

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.

Publications

Journal Articles

Arrasmith, A. T., P. J. Czarnik, P. J. Coles and L. Cincio. Error Mitigation with Clifford quantum-circuit data. Submitted to *Physical Review Letters*. (LA-UR-20-23755)

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. J., 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. Submitted to *arXiv+PRB*. (LA-UR-20-29946)

Lowe, A. J., M. E. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, L. Cincio and P. J. Coles. Unified approach to data-driven error mitigation. Submitted to *arXiv+Physical Review X Quantum*. (LA-UR-20-28845)

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)

Presentation Slides

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)

Error Correction and Speed-up of Near-term Quantum Computing Architectures

Patrick Coles
20200677PRD1

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

Journal Articles

Pesah, A., M. V. S. Cerezo de la Roca, S. Wang, T. J. Volkoff, A. T. Sornborger and P. J. Coles. Absence of Barren Plateaus in Quantum Convolutional Neural Network. Submitted to *Physical Review X*. (LA-UR-20-29031)

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. and P. J. Coles. Large gradients via correlation in random parameterized quantum circuits. 2021. *Quantum Science and Technology*. **6** (2): 25008. (LA-UR-20-23818 DOI: 10.1088/2058-9565/abd891)

Quantum Simulation of Quantum Field Theories

Rolando Somma
20200678PRD1

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.

Publications

Journal Articles

Sahinoglu, M. B., D. Williamson, N. Bultinck, M. Marien, J. Haegeman, N. Schuch and F. Verstraete. Characterizing topological order with matrix product operators. Submitted to *Annales Henri Poincare*. (LA-UR-20-29927)

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. and R. D. Somma. Hamiltonian simulation in the low energy subspace. . (LA-UR-20-27396)

Neuromorphic Memcomputing via Interacting Nanomagnets

Francesco Caravelli
20170660PRD1

Project Description

The brain is estimated to perform up to E+14 TEPS (Traversed Edge Per Second) at a cost of approximately 20-25 Watts. The DOE BlueGene performs roughly E +13 TEPS, at a cost of roughly E+6 Watts. We propose to overcome that limitation via memcomputing. The concept of mem-computing is a more general approach to beyond-Turing-machine computation that has been identified by DOE as an essential national security challenge.

Technical Outcomes

The project has been successful in delivering two new frameworks to study computation and neuromorphic computing in Physical systems. In the context of Artificial Spin Ice, the team has shown that both logical gates and memristors can be obtained via connected magnetic nanoislands due to the Anisotropic Magnetoresistance effect in permalloy. In the context of memristor networks, this project shows that these can be mapped to the disordered Ising models and topological Hopfield networks.

Publications

Journal Articles

*Caravelli, F. Locality of interactions for planar memristive circuits. 2017. *Physical Review E*. **96** (5): 052206. (LA-UR-17-23533 DOI: 10.1103/PhysRevE.96.052206)

Caravelli, F. Asymptotic behavior of memristive circuits and combinatorial optimization. Submitted to *Proceeding of the National Academy of Science*. (LA-UR-17-30617)

*Caravelli, F. Asymptotic Behavior of Memristive Circuits. 2019. *Entropy*. **21** (8): 789. (LA-UR-18-24748 DOI: 10.3390/e21080789)

Caravelli, F. On a ``continuum" formulation of the Ising model partition function. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-19-28192)

Caravelli, F. Spin-Dot interactions in Artificial Spin Ice: population inversion as an entropic effect. Submitted to *Physical Review Letters*. (LA-UR-19-31351)

Caravelli, F., C. Nisoli and G. Chern. Phase-change spin ice memory resistor. Submitted to *Physical Review Letters*. (LA-UR-19-27438)

*Caravelli, F., G. Coulter-De Wit, L. P. Garcia-Pintos and A. Hamma. Random quantum batteries. 2020. *Physical Review Research*. **2** (2): 023095. (LA-UR-19-28177 DOI: 10.1103/PhysRevResearch.2.023095)

Caravelli, F. and C. Nisoli. Computation via Interacting Magnetic Memory Bites: Integration of Boolean Gates. Submitted to *Physical Review X*. (LA-UR-18-23268)

*Caravelli, F. and J. P. Carbajal. Memristors for the Curious Outsiders. 2018. *Technologies*. **6** (4): 118. (LA-UR-18-27766 DOI: 10.3390/technologies6040118)

*Caravelli, F. and P. Barucca. A mean-field model of memristive circuit interaction. 2018. *EPL (Europhysics Letters)*. **122** (4): 40008. (LA-UR-17-23729 DOI: 10.1209/0295-5075/122/40008)

Cooper, F. M. Universal scaling and ferroelectric hysteresis regimes in the giant squid axon propagating action potential: a Phase Space Approach. Submitted to *Physical Review E*. (LA-UR-17-30245)

*Cui, T., F. Caravelli and C. Ududec. Correlations and clustering in wholesale electricity markets. 2018. *Physica A: Statistical Mechanics and its Applications*. **492**: 1507-1522. (LA-UR-17-26648 DOI: 10.1016/j.physa.2017.11.077)

McNerney, J., F. Caravelli, C. Savoie and J. D. Farmer. The network structure of the economy amplifies secular growth. Submitted to *Nature*. (LA-UR-17-22598)

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)

Sheldon, F. C., F. Caravelli and A. Kolchinsky. The Computational Capacity of Memristor Reservoirs. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-26991)

*Zegarac, A. and F. Caravelli. Memristive networks: From graph theory to statistical physics. 2019. *EPL (Europhysics Letters)*. **125** (1): 10001. (LA-UR-18-31372 DOI: 10.1209/0295-5075/125/10001)

Presentation Slides

Caravelli, F. Non-equilibrium properties of memristive networks. Presented at *Applied Statistical Physics*, Santa Fe, New Mexico, United States, 2017-05-01 - 2017-05-05. (LA-UR-17-23642)

Caravelli, F. Information Theory and (F)RG. Presented at *FRG Conference*, Trento, Italy, 2019-09-16 - 2019-09-16. (LA-UR-19-29327)

Caravelli, F. Memristive Networks. Presented at *Talk @ICTP Trieste*, Trieste, Italy, 2019-09-23 - 2019-09-23. (LA-UR-19-29539)

Optimal Control of Quantum Machines

Davide Girolami
20180702PRD1

Project Description

The goal of the project is to reach a full understanding of the correlation structures in many-body quantum systems, and employ this knowledge to control quantum devices in realistic conditions. Quantum devices are expected to revolutionize data processing. Specifically, quantum computers will outperform the most powerful supercomputers in terms of speed. The project will study how to improve their efficiency, making them more robust to noise sources. A potential application of this new kind of device is the ultrafast simulation of nuclear experiments, made possible by exploiting the peculiar properties of quantum systems. This will help to efficiently maintain and steward the nuclear stockpile, a key challenge of relevance for national security. Another potential use of the project results may be in efficient long-distance quantum communication networks, enabling the transfer of sensitive data shielded from non-authorized access.

Technical Outcomes

The first important result of the project is the exact calculation of the minimum energy and time required for experimentally creating quantum correlations, such as entanglement. This finding advances our understanding of quantum processes, improving our ability to run quantum computers more efficiently. A second significant result is a quantum algorithm for discovering causal relations in complex data sets. The protocol paves the way for harnessing quantum causal links as a resource for quantum technologies.

Publications

Journal Articles

*Girolami, D. How Difficult is it to Prepare a Quantum State?. 2019. *Physical Review Letters*. **122** (1): 010505. (LA-UR-18-27400 DOI: 10.1103/PhysRevLett.122.010505)

Girolami, D. Quantifying Causation. Submitted to *Physical Review Letters*. (LA-UR-19-26319)

*Yadin, B., P. Bogaert, C. E. Susa and D. Girolami. Coherence and quantum correlations measure sensitivity to dephasing channels. 2019. *Physical Review A*. **99** (1): 012329. (LA-UR-18-29513 DOI: 10.1103/PhysRevA.99.012329)

Presentation Slides

Girolami, D. Detecting metrologically useful asymmetry and entanglement by a few local measurements.. Presented at *SQUINT Workshop*, Santa Fe, New Mexico, United States, 2018-02-22 - 2018-02-22. (LA-UR-18-21362)

Girolami, D. Characterizing genuine multipartite correlations and their pattern complexity. Presented at *APS March Meeting 2018*, Los Angeles, California, United States, 2018-03-05 - 2018-03-05. (LA-UR-18-21555)

Girolami, D. Characterizing genuine multipartite correlations and their pattern complexity. Presented at *ICCS 2018*, Cambridge, Massachusetts, United States, 2018-07-22 - 2018-07-22. (LA-UR-18-26801)

Girolami, D. Characterizing genuine multipartite correlations and their pattern complexity. Presented at *Information Engines at the Frontiers of Nanoscale Thermodynamics*, Telluride, Colorado, United States, 2018-07-19 - 2018-07-26. (LA-UR-18-26800)

Girolami, D. Quantum Resources for Information Processing. . (LA-UR-19-20054)

Girolami, D. Quantum Resources for Information Processing. . (LA-UR-19-20055)

Girolami, D. Quantum Resources for Information Processing. . (LA-UR-19-21941)

Girolami, D. A Quantum Law of Requisite Variety. Presented at *APS March Meeting 2019*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-21940)

Girolami, D. How difficult is it to [re[are a quantum state?. . (LA-UR-19-23651)

Girolami, D. Quantum Resources for Noisy Information Processing. . (LA-UR-19-24297)

Girolami, D. Quantum Resources for Noisy Information Processing. . (LA-UR-19-27815)

Machine Learning of Membrane Transport of Signals and Drugs

Sandrasegaram Gnanakaran
20180745PRD3

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 molecular-level understanding of the operating principles governing how antibiotics move across membranes. The combined approach of multi-scale mathematical models and machine learning proposed in this project is not limited to biological system, but rather can be applied to understand other multi-scale problems of interest to DOE/NNSA. For example, the biological membrane for which the model is being developed have complexities very similar to those found in the properties of materials and our modeling procedure could be applied to detect defects in materials. The integration of above approach with high performance computing help solidify DOE's exascale computing initiatives, thereby strengthening the key NNSA goal of stockpile stewardship.

Technical Outcomes

The project identified a "chemical vocabulary" for drug permeation of bacterial membranes. The project created an algorithm called "Hunting FOX" for "Hunting Fragments Of X," with which the team identified the pieces of molecules known to permeate the impermeable outer membranes of Gram negative bacteria. The algorithm developed is generalizable to other systems of interest. The team also developed machine learning models describing ways different classes of molecules interact with bacteria.

Publications

Journal Articles

Lindsay, R. J., R. A. Mansbach, T. Shen and S. Gnanakaran. Effects of pH on an IDP conformational ensemble explored by molecular dynamics simulation. 2021. *Biophysical Chemistry*. 106552. (LA-UR-20-30442 DOI: 10.1016/j.bpc.2021.106552)

Mansbach, R. A., C. A. Lopez Bautista, N. W. Hengartner, G. Malloci, J. Mehla, I. V. Leus, P. Ruggerone, H. I. Zgurskaya, V. Rybenkov and S. Gnanakaran. Application of a Fragment-Based Algorithm for Drug Design to Antibiotics for Resistant Bacteria. Submitted to *Nature Communications*. (LA-UR-19-24832)

*Mansbach, R. A., I. V. Leus, J. Mehla, C. A. Lopez, J. K. Walker, V. V. Rybenkov, N. W. Hengartner, H. I. Zgurskaya and S. Gnanakaran. Machine Learning Algorithm Identifies an Antibiotic Vocabulary for Permeating Gram-Negative Bacteria. 2020. *Journal of Chemical Information and Modeling*. **60** (6): 2838-2847. (LA-UR-20-22055 DOI: 10.1021/acs.jcim.0c00352)

Mansbach, R. A., S. Chakraborty, T. K. Nguyen and S. Gnanakaran. Differential molecular signatures of the D and G forms the SARS-CoV2 trimeric Spike protein. Submitted to *Science Advances*. (LA-UR-20-25181)

*Mansbach, R. A., T. Travers, J. M. Fair and S. Gnanakaran. Snails In Silico: A Review of Computational Studies on the Conopeptides. 2019. *Marine Drugs*. **17** (3): 145. (LA-UR-19-21315 DOI: 10.3390/md17030145)

*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)

Mehla, J., G. Malloci, R. A. Mansbach, C. A. Lopez Bautista, P. D. Manrique Charry, R. Tsivkovski, S. B. Grindstaff, R. H. Cascella, N. W. Hengartner, L. K. Herndon, A. Atzori, A. V. Vargiu, F. Cardamone, O. Lomovskaya, P. Ruggerone, S. Gnanakaran, V. V. Rybenkov and H. I. Zgurskaya. Physico-chemical and molecular descriptors of efflux substrates, inhibitors and avoiders in Pseudomonas aeruginosa. Submitted to *ACS Infectious Diseases*. (LA-UR-20-21086)

*Shmilovich, K., R. A. Mansbach, H. Sidky, O. E. Dunne, S. S. Panda, J. D. Tovar and A. L. Ferguson. Discovery of Self-Assembling \xcf\x80-Conjugated Peptides by Active Learning-Directed Coarse-Grained Molecular Simulation. 2020. *The Journal of Physical Chemistry B*. **124** (19): 3873-3891. (LA-UR-19-27326 DOI: 10.1021/acs.jpcb.0c00708)

Reports

Travers, T., R. A. Mansbach, B. H. Mcmahon, J. M. Fair and S. Gnanakaran. Evaluating the evolutionarily-optimized combinatorial peptide libraries of cone snails from a structural perspective. Unpublished report. (LA-UR-18-25722)

Presentation Slides

Mansbach, R. A., C. A. Lopez Bautista, N. W. Hengartner and S. Gnanakaran. A Fragment Library for Drug Activity in Gram Negative Bacteria. . (LA-UR-19-20062)

Toward Automated Interpretation of Large, High Resolution Computed Tomography Volumes

Christopher Stull
20200485MFR

Project Description

The use of Computed Tomography (CT or, in the medical field, CAT scan) as an inspection modality for weapons' components has seen a dramatic increase during the past decade, and especially during the past five years. The efficiency of CT interpretation is largely driven by staff availability and computing resources, due to the labor-dependent state-of-the-practice of staff manually examining 100s to 1000s of images. Thus far, automated interpretation of large, high resolution CT volumes, in particular, has proven difficult even with modern, commercially-available visualization software and cutting edge computing resources. Technological advances have made such large, high resolution CT volumes more readily attainable in terms of the Los Alamos Stockpile Stewardship mission, which necessitates research and development efforts to insure CT interpretation does not become a substantial bottleneck in the inspection process. The present proposal aims to address this potential shortcoming by leveraging PetaVision, a neural simulation toolbox developed at Los Alamos over the past decade, that has a proven track record of image classification on institutional class computing systems (e.g. Trinity). This effort is expected to yield a semi-automated means by which large, high resolution CT volumes may be interpreted with limited input by staff.

Launch Vehicle Detection and Tracking System

John Scott
20200664DI

Project Description

This proposed project is a first step to implementing a resilient architecture to address the Find-Fix-Track portion of the military’s target kill chain (Find-Fix-Track-Target-Engage-Assess). The proposed system will be capable of detecting the launch of a target-of-interest, tracking the target's trajectory, and predicting its destination. This system will provide early warning of potential threats to warfighters and provide critical information for intercepting these vehicles before they reach their intended target.

Publications

Presentation Slides

Durham, J. M. and R. T. Thornton. Director's Initiative LDRD: Launch Vehicle Detection and Tracking 20200664DI. . (LA-UR-20-30319)

Artificial Intelligence for Sensing

Aric Hagberg
20200669DI

Project Description

This project addresses national security challenges in sensing by exploring and developing modern artificial intelligence (AI) algorithms for use at sensor locations. Sensors typically have limited computing capability and are unsuitable for complicated compute-intense algorithms. New AI techniques such as deep learning, can exploit limited computing by using a combination of high performance computing for training algorithms on large existing data sets and lower-performance computing at the sensor that use the trained algorithms for analysis or prediction. The expected outcomes of this research project are identification of sensor challenges where Los Alamos has significant strategic opportunity to create advantages with AI, creation of new interdisciplinary teams and new communities of researchers connecting AI experts with engineers and sensor experts, and development of one or more technology advances using AI/Machine Learning algorithms for sensing in a Los Alamos application. National security mission applications with high potential for AI impact are: satellite and remote collection, additive manufacturing, cyber-physical security, and data analysis at scientific user facilities.

Publications

Presentation Slides

Oyen, D. A., C. M. Sweeney, J. L. Barber, K. M. Mertes and N. Panda. Deep Learning to Accelerate Ptychography: AI@Sensor Rapid Response. . (LA-UR-20-27401)

Reinisch, E. C., C. X. Ren, A. F. Roberts, C. J. Wilson, P. B. Eriksson and A. Ziemann. Remote sensing of polar ice: combining synthetic aperture radar and machine learning for operational navigability. Presented at *SPIE Defense +Commercial Sensing 2021*, (virtual), New Mexico, United States, 2021-04-12 - 2021-04-16. (LA-UR-21-22747)

Sweeney, C. M. Deep Learning-Assisted Image Reconstruction of Scanned Samples from X-ray Diffraction (XRD) (A.K.A. Ptychography). . (LA-UR-21-22122)

Quantum Algorithm Development for Optimization

Stephan Eidenbenz
20200671DI

Project Description

The quantum optimization project will develop novel and analyze existing quantum computing algorithms used for optimization problems that occur in various mission areas, such as optimum satellite or sensor placement for event detection in non-proliferation activities and process scheduling problems in high-performance computing in the stockpile stewardship mission. Quantum computing algorithms have the potential to outperform their classical counterparts significantly and thus have the potential to overcome current strategic computing limits. We aim to identify and quantify from a theoretical and experimental perspective the advantage that quantum optimization can achieve over classical-only optimization. Our approach will combine follow along two tracks: In an experimental track, where we run experiments on various Noisy Intermediate-Scale Quantum (NISQ) Devices, such as our own D-Wave quantum annealer, the International Business Machines (IBM) Quantum computer; in the theoretical track, this project will mathematically proof performance bounds of existing optimization algorithms and use these insights to develop novel provable quantum optimization algorithms.

Publications

Journal Articles

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Vuffray, M. D., C. J. Coffrin, Y. A. Kharkov and A. Lokhov. Programmable Quantum Annealers as Noisy Gibbs Samplers. Submitted to *Science*. (LA-UR-20-28047)

Conference Papers

Baertschi, A. and S. J. Eidenbenz. Grover Mixers for QAOA: Shifting Complexity from Mixer Design to State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Broomfield, Colorado, United States, 2020-10-12 - 2020-10-16). (LA-UR-20-23893)

Presentation Slides

Baertschi, A., S. J. Eidenbenz and J. Cook. The Quantum Alternating Operator Ansatz on Maximum k-Vertex Cover. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28067)

Baertschi, A., S. J. Eidenbenz and J. Cook. The Quantum Alternating Operator Ansatz on Maximum k-Vertex Cover. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28072)

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Baertschi, A. and S. J. Eidenbenz. Grover Mixers for QAOA: Shifting Complexity from Mixer Design to State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28071)

Vuffray, M. D., A. Lokhov, C. J. Coffrin and J. A. Nelson. Programmable Quantum Annealers as Noisy Boltzmann Samplers. Presented at *D-Wave Qubits 2020*, online, New Mexico, United States, 2020-09-28 - 2020-09-29. (LA-UR-20-27111)

Posters

Baertschi, A. and S. J. Eidenbenz. Grover Mixer QAOA: Feasible State Superpositions, Convergence to Optimum, and Limitations. Presented at *24th Annual Conference on Quantum Information Processing QIP 2021*, Munich, Germany, 2021-02-01 - 2021-02-05. (LA-UR-21-20773)

Trustworthy and Reliable Machine Learning

Juston Moore
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Project Description

Ensuring the trustworthiness of artificial intelligence (AI) is imperative for making AI safe to deploy in the real world, especially for national security applications. This Director's Initiative project aims to ensure that AI can be understood and trusted by analysts, will perform reliably under expected conditions and exhibit robust behavior in unfamiliar domains, and will remain resilient both in the presence of malicious adversaries and under real-world uncertainty. AI is now being deployed for security purposes by governments around the world. However, current AI technology is plagued by known vulnerabilities, which can cause systems to fail in unpredictable and potentially catastrophic ways. This project will demonstrate novel approaches to constructing and vetting AI that emphasize trustworthiness in real-world situations. Recent advances at Los Alamos promise strategies for developing a more trustworthy AI. Based on this foundation, our core hypothesis is that trustworthy AI can be constructed by first modeling the deep structure of the data, which is inherent in scientific data, to ensure that AI does not rely on superficial features but rather depends upon perceptually-salient components of the data. This Director's Initiative project will contribute methods for ensuring that AI deployed at Los Alamos is suitable for critical applications.

Technical Outcomes

This project funded broad capability growth supporting multiple mission areas. The research included 1) an improved chemical composition discovery method from laser-induced breakdown spectroscopy (LIBS) ChemCam data, 2) an improved dataset for radio frequency modulation detection, 3) novel methods for reliable deepfake image detection, and 4) innovative lattice-based methods for hardening machine learning classifiers. This project also supported workforce development by funding three student internships and building a JupyterHub server to supporting agile data science workflows from home.

Publications

Journal Articles

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Kim, E., J. Rego, Y. Z. Watkins and G. Kenyon. Modeling Biological Immunity to Adversarial Examples. Presented at *CVPR*. (Seattle, Washington, United States, 2020-06-16 - 2020-06-16). (LA-UR-20-24457)

Moore, J. S. and H. T. Jones. 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)*. (Vancouber, Canada, 2020-12-12 - 2020-12-12). (LA-UR-20-29898)

T. Nguyen-Fotiadis, N. T., J. S. Moore and G. Kenyon. Using models of cortical development based on sparse coding to discriminate between real and synthetically generated faces. Presented at *NeurIPS*. (Los Alamos, New Mexico, United States, 2020-12-06 - 2020-12-06). (LA-UR-20-24451)

Teti, M. A., E. E. Meyer and G. Kenyon. Can lateral inhibition for sparse coding help explain V1 neuronal responses to natural stimuli?. Presented at *Southwest Symposium on Image Analysis and Interpretation (SSIAI)*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29). (LA-UR-20-22286)

Wang, D. A., C. S. M. Strauss, J. M. Springer, A. M. Thresher, H. P. J. Pritchard and G. Kenyon. Sparse MP4. Presented at *Southwest Symposium on Image Analysis and*

Interpretation (SSIAI). (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29). (LA-UR-20-22060)

Zhang, D. Y., G. J. Kunde, M. A. Teti, J. S. Moore and B. J. Migliori. Detecting Adversarial Attacks on Speech Recognition with Voice Recognition. Presented at *49th Annual IEEE AIPR 2020: Trusted Computing, Privacy, and Securing Multimedia*. (Washington DC, District Of Columbia, United States, 2020-11-15 - 2020-11-21). (LA-UR-20-29457)

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Burroughs, S. J., E. S. Michalak, J. S. Moore and G. Kenyon. Analysis of Low and High Frequency Bands in Deepfake Detection. . (LA-UR-20-25932)

Burroughs, S. J., E. S. Michalak, J. S. Moore and G. Kenyon. Analysis of Low and High Frequency Bands in Deepfake Detection. . (LA-UR-20-26121)

Eren, M. E., J. S. Moore and B. Alexandrov. Anomalous Event Detection using Non-Negative Poisson Tensor Factorization. . (LA-UR-20-25933)

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Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics (ISI)*, Online, New Mexico, United States, 2020-11-09 - 2020-11-10. (LA-UR-20-28568)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-10. (LA-UR-20-28561)

Jones, H. T. and J. S. Moore. Detecting Deepfakes with VQVAEs. . (LA-UR-20-25898)

Mehta, A., C. Scott, D. A. Oyen, N. Panda and G. Srinivasan. Physics-Informed Spatiotemporal Deep Learning for Emulating Coupled Dynamical Systems. Presented at *AAAI Symposium on Machine Learning for Physical Sciences*, Palo Alto, California, United States, 2020-03-23 - 2020-03-23. (LA-UR-20-22513)

Moore, J. S., G. Kenyon, B. J. Migliori, A. M. Thresher, E. S. Michalak, M. J. Dixon, N. T. T. Nguyen-Fotiadis and P. T. Hraber. Adversarially Robust Sparse Coding for GAN Detection. Presented at *Naval Applications of Machine Learning*, San DIego, California, United States, 2020-02-25 - 2020-02-25. (LA-CP-20-20335)

Najt, L. S., M. J. Dixon, N. W. Lemons and J. S. Moore. Leveraging computational hardness in adversarial machine learning. . (LA-UR-20-25949)

Najt, L. S., M. J. Dixon, N. W. Lemons and J. S. Moore. Leveraging computational hardness in adversarial machine learning. . (LA-UR-20-25949)

Oyen, D. A. Transductive Learning with Graphical Models: Characterizing Adversarial Data in the Wild. Presented at *Applied Imagery Pattern Recognition*, virtual, New Mexico, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-27836)

Prasad, R. C. and J. S. Moore. Bootstrapping Datasets for Deepfake Detection. . (LA-UR-20-25917)

Zhang, D. Y., G. J. Kunde, M. A. Teti, J. S. Moore and B. J. Migliori. Detecting Adversarial Attacks on Speech Recognition with Voice Recognitio. Presented at *49th Annual IEEE AIPR 2020: Trusted Computing, Privacy, and Securing Multimedia*, Washington DC, District Of Columbia, United States, 2020-10-13 - 2020-10-15. (LA-UR-20-28138)

Zhang, D. Y. and B. J. Migliori. Improving Robustness to Audio Perturbations Using Biological Receptive Fields. . (LA-UR-20-25906)

Zhang, D. Y. and B. J. Migliori. Improving Robustness of Audio Perturbations Using Biological Receptive Fields. . (LA-UR-20-26149)

Posters

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)

Advanced Algorithms for Multiphysics Applications on Modern Computer Architectures

Christopher Werner
20200670DI

Project Description

Hydrodynamics modeling is critical to Los Alamos National Laboratory (LANL) core missions. This mission-critical area at LANL will benefit from investments in developing and implementing high-order hydrodynamic methods that can be coupled to existing LANL production codes. The methods currently used in the Advanced Simulation and Computing (ASC) codes have their origins in work following World War II and are in most cases low-order, so they scale poorly and offer little hope for high-fidelity simulations of non-linear physics problems. Recent years have seen the growth of higher order methods in other institutions because of their increased accuracy and adaptability to modern Graphic Processing Unit (GPU) architectures. This project aims to develop a higher-order hydrodynamic scheme within a production code framework–free Lagrange (FLAG)– that can be expected to scale well on modern computer architectures. The project will also develop a framework for higher-order schemes and implement a scheme on that framework in the production code Radiation Adaptive Grid Eulerian (known as "xRAGE" at LANL). This would form the basis for an advanced hydrodynamics code that (a) can be used to simulate multi-material, multi-physics problems with scale-bridging advanced material models, and that (b) performs well on modern computer architectures.

Technical Outcomes

For the Lagrangian goals, the feasibility of high order Lagrangian discontinuous Galerkin (DG) hydrodynamics was demonstrated. For the Eulerian goals of the project, briquette adaptive mesh refinement (AMR) methods were implemented in two and three dimensions. The numerical methods are new and most advanced in the scientific community. The briquette AMR and numerical methods could be together or separately used in the community, including the Advanced Simulation and Computing (ASC) program.

Publications

Presentation Slides

Burton, D. E. High order discontinuous Galerkin (DG) hydrodynamics for the FLAG code. Presented at *XCP Seminar*, Los Alamos, New Mexico, United States, 2020-08-27 - 2020-08-27. (LA-UR-20-27045)

Machine Learning Enhanced Modeling

Enrique Batista
20200001CR

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.

Publications

Journal Articles

DeSantis, D. F., P. J. J. Wolfram, K. E. Bennett and B. Alexandrov. Coarse-Grain Cluster Analysis of Tensors With Application to Climate Biome Identification. Submitted to *IOP - Machine Learning: Science and Technology*. (LA-UR-20-20548)

Lovell, A. E., A. T. Mohan, P. Talou and M. Chertkov. Quantified uncertainties in fission yields from machine learning. *EPJ Web of Conferences*. **242**: 05003. (LA-UR-19-31677 DOI: 10.1051/epjconf/202024205003)

Lovell, A. E., A. T. Mohan and P. Talou. Quantifying Uncertainties on Fission Fragment Mass Yields with Mixture Density Networks. Submitted to *Journal of Physics G: Nuclear and Particle Physics*. (LA-UR-20-22632)

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Lovell, A. E., P. Talou, I. Stetcu and K. J. Kelly. Correlations Between Fission Fragment and Neutron Anisotropies in Neutron-Induced Fission. Submitted to *Physical Review C*. (LA-UR-20-22603)

R. Metivier, D. M., M. D. Vuffray and S. Misra. Efficient Polynomial Chaos Expansion for Uncertainty Quantification in Power Systems. Submitted to *Electric Power Systems Research*. (LA-UR-19-30262)

Nelson, T. R., B. T. Nebgen, A. J. White, Y. Zhang, H. Song, J. A. Bjorgaard, A. E. Sifain, B. Rodriguez-Hernandez, V. M. Freixas, S. Fernandez-Alberti, A. Roitberg, W. F. I. Malone and S. Tretiak. NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22362)

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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Srinivasan, S. and N. Panda. What is the gradient of a scalar function of a symmetric matrix ?. Submitted to *SIAM Journal on Matrix Analysis and Applications*. (LA-UR-19-31267)

Yang, H., D. P. Morton and D. Duque. Optimizing Diesel Fuel Supply Chain Operations for Hurricane Relief. Submitted to *IIE Transactions*. (LA-UR-20-23789)

Yang, H., O. Surer, D. Duque, D. P. Morton, B. Singh, S. J. Fox, R. Pasco, K. Pierce, P. Rathouz, Z. Du, M. Pignone, M. E.

Escott, S. I. Adler, S. C. Johnston and L. A. Meyers. Design of COVID-19 Staged Alert Systems to Ensure Healthcare Capacity with Minimal Closures. Submitted to *Science*. (LA-UR-20-29654)

Zhou, G., B. T. Nebgen, N. E. Lubbers, W. F. I. Malone, A. M. Niklasson and S. Tretiak. GPU-Accelerated Semi-Empirical Born Oppenheimer Molecular Dynamics using PyTorch. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22394)

Conference Papers

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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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Presentation Slides

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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)

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Rapid Response: Novel Computing

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20180719CR

Project Description

The computational scalability of traditional computer hardware has stalled because miniaturization has reached a level, where quantum mechanical effects can no longer be ignored. Developing novel computing technologies, such as quantum computing, neuromorphic computing, and application-specific designs is crucial to retain the nation's technological edge. Our rapid response project will explore the near-term opportunities that these technologies offer.

Technical Outcomes

The Rapid Response project was comprised of about 18 tasks each of which lasted less than a full fiscal year. The technical outcomes contribute significantly to our understanding in these fields. Some of the highlights include an improved bound on the quantum resources required to verify the solution of a linear system of equations, improved quantum tomography, using quantum annealers as noisy Boltzmann samplers, and treating quantum spin ice systems with quantum annealers

Publications

Journal Articles

Caravelli, F., C. Nisoli and G. Chern. Phase-change spin ice memory resistor. Submitted to *Physical Review Letters*. (LA-UR-19-27438)

Jayakumar, A., A. A. Adedoyin, J. J. Ambrosiano, P. M. Anisimov, A. Baertschi, W. R. Casper, G. Chennupati, C. J. Coffrin, H. N. Djidjev, D. O. Gunter, S. Karra, N. W. Lemons, S. Lin, A. Malyzhenkov, D. D. L. Mascarenas, S. M. Mniszewski, B. T. Nadiga, D. O'Malley, D. A. Oyen, S. D. Pakin, L. Prasad, R. M. Roberts, P. R. Romero, N. Santhi, N. Sinitsyn, P. J. Swart, J. G. Wendelberger, B. Yoon, R. J. Zamora, W. Zhu, S. J. Eidenbenz, P. J. Coles, M. D. Vuffray and A. Lokhov. Quantum Algorithm Implementations for Beginners. Submitted to *ACM Transactions on Quantum Computing*. (LA-UR-20-22353)

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Henke, K. G., B. J. Migliori and G. Kenyon. Machine Learning in a Post Moore's Law World: Quantum vs. Neuromorphic Substrates. Presented at *IEEE Southwest Symposium on Image Analysis and Interpretation (SSIAI)*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-31). (LA-UR-20-22291)

Hijazi, H. L. Perspective Envelopes for Bilinear Functions. Presented at *LeGO 2018 - Int. Workshop on Global Optimization*. (Leiden, Netherlands, 2018-09-17 - 2018-09-17). (LA-UR-18-27814)

Jayakumar, A., A. Lokhov, S. Misra and M. D. Vuffray. Learning of Discrete Graphical Models with Neural Networks. Presented at *NeurIPS*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-24927)

Mniszewski, S. M., R. Shaydulin, H. M. Ushijima-Mwesigwa, I. Safro and Y. Alexeev. Community Detection Across Emerging Quantum Architectures. Presented at *3RD INTERNATIONAL WORKSHOP ON POST-MOORE'S ERA SUPERCOMPUTING (PMES) - Supercomputing 2018*. (Dallas, Texas, United States, 2018-11-11 - 2018-11-16). (LA-UR-18-28413)

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Somma, R. D., M. B. Sahinoglu and S. Gu. Fast-forwarding quantum evolution. Presented at *QIP*. (Munich (Online), Germany, 2021-02-01 - 2021-02-05). (LA-UR-20-29591)

Presentation Slides

Coffrin, C. J. Combinatorial Optimization on D-Wave. . (LA-UR-18-25316)

Coffrin, C. J. Harnessing Analog Noise: A Hybrid Algorithm for Binary Quadratic Optimization with Uncertainty. . (LA-UR-19-24684)

Coffrin, C. J. The Potential of Quantum Annealing for Rapid Solution Structure Identification. . (LA-UR-20-21046)

Coffrin, C. J. The Performance of Corrupted Biased Ferromagnets on D-Wave's 2000Q. Presented at *Qubits 2020*, Online, New Mexico, United States, 2020-09-28 - 2020-09-29. (LA-UR-20-26831)

Coffrin, C. J., S. Misra, M. D. Vuffray and J. A. Nelson. Demonstrating the Computational Value of Noisy Boltzmann Samplers. . (LA-UR-20-27170)

DeStefano, Z. L. Distributed and Verifiable Machine Learning using Zero-Knowledge Proofs. . (LA-UR-20-25976)

DeStefano, Z. L. Distributed and Verifiable Machine Learning using Zero-Knowledge Proofs. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-26182)

DeStefano, Z. L. Privacy Preserving, Distributed, and Verifiable Machine Learning for COVID-19 Identification using Zero-Knowledge Proofs. Presented at *Chesapeake Large-Scale Analytics Conference (CLSAC)*, Annapolis, Maryland, United States, 2020-10-06 - 2020-10-06. (LA-UR-20-27590)

Dixon, M. J. and Z. L. DeStefano. Distributed, Private, and Verifiable Neural Networks using Zero-knowledge Proofs. Presented at *Lab Research Technical Exchange*, Los Alamos, New Mexico, United States, 2021-01-26 - 2021-01-26. (LA-UR-21-20646)

Green, A. W. and D. D. L. Mascarenas. Fast Digital Coded Exposure for the Silicon Retina. . (LA-UR-20-25253)

Kintner, J. A., N. P. Symons, J. K. MacCarthy and J. D. Carmichael. Formulating the Seismic Association Problem Using Graph Theory, Applications to Estimating an Efficient Solution with Quantum Computers. Presented at *AGU 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29391)

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Lokhov, A. Sample-optimal Learning of Graphical Models (and opening the D-Wave annealer's quantum box). Presented at *Statistical physics and machine learning back together*, Cargese, France, 2018-08-20 - 2018-08-20. (LA-UR-18-29149)

Mniszewski, S. M., C. F. A. Negre, J. P. Terry and P. D. Akrobotu. Quantum Isomer Search. . (LA-UR-19-29554)

Mniszewski, S. M., C. F. A. Negre and H. M. Ushijima-Mwesigwa. Graph Clustering Approaches using Near-term Quantum Computing. Presented at *2018 Quantum Computing Workshop*, Lemont, Illinois, United States, 2018-07-25 - 2018-07-27. (LA-UR-18-26831)

Mniszewski, S. M., C. F. A. Negre and H. M. Ushijima-Mwesigwa. Graph Clustering Approaches using Quantum Annealing. Presented at *D-Wave Users Conference Qubits 2018*, Knoxville, Tennessee, United States, 2018-09-24 - 2018-09-27. (LA-UR-18-28859)

Mniszewski, S. M., C. F. A. Negre and H. M. Ushijima-Mwesigwa. Hybrid Quantum Computing for Graph Partitioning and Community Detectionn. . (LA-UR-18-29049)

Mniszewski, S. M., H. M. Ushijima-Mwesigwa, C. F. A. Negre and I. Safro. Multilevel Quantum Annealing for Graph Partitioning. Presented at *Quantum Computing Workshop, Argonne National Laboratory*, Lemont, Illinois, United States, 2018-07-25 - 2018-07-27. (LA-UR-18-27179)

Mniszewski, S. M., H. M. Ushijima-Mwesigwa, C. F. A. Negre and I. Safro. Multilevel Quantum Annealing for Graph Partitioning. Presented at *D-Wave Users Conference Qubits*

2018, Knoxville, Tennessee, United States, 2018-09-24 - 2018-09-27. (LA-UR-18-29051)

Mniszewski, S. M., P. D. Akrobotu and J. P. Terry. Combinatorics Algorithms on Near-term Quantum Architectures. . (LA-UR-19-27040)

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Somma, R. D. Quantum algorithms for systems of linear equations. Presented at *2020 Quantum Summer Symposium*, Los Angeles, California, United States, 2020-07-22 - 2020-07-23. (LA-UR-20-25084)

Sornborger, A. T., A. F. M. V. Renner, F. C. Sheldon, A. V. Zlotnik and L. Tao. A Pulse-Gated, Spiking Neural Implementation of the Backpropagation Algorithm. Presented at *Conference on Data Analysis (CoDA) 2020*, Santa Fe, New Mexico, United States, 2020-02-26 - 2020-02-26. (LA-UR-20-21875)

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Wang, Z. and T. Li. Quantum computing using ultracolde neutrons (UCN). . (LA-UR-19-30745)

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Henke, K. G., B. J. Migliori and G. Kenyon. Quantum vs Neuormorphic: The Battle for Post Moore's Law Computation. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21481)

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L. Mascarenas, D. D., A. W. Green, J. E. Morales Garcia, A. Cattaneo and M. Anghel. Summer 2020 Imager Dynamics Dataset. Dataset. (LA-UR-20-26006)

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Materials for the Future

Uncovering the Role of 5f-electron Magnetism in the Electronic Structure and Equation of State of Plutonium

Neil Harrison
20180025DR

Project Description

Accurate simulations of plutonium under extreme conditions require an accurate knowledge of the electronic structure and equation of state. Magnetism is presently a missing component of the electronic structure and equation of state that is known to have a significant influence on the equilibrium volume, bulk modulus and other properties. The goal of the present project is to determine primarily by way of experiment, accompanied by advanced theoretical modeling tools, the correct way of incorporating the effects of magnetism in the electronic structure and equation of state of plutonium. The end result will be an accurate understanding of the mechanism at play when delta-plutonium undergoes its initial volume collapse at low pressure. Such an understanding is crucial for accurate estimates to be made of plutonium's physical quantities under reduced volume, and also by extrapolation into more extreme environments where accurate or safe measurements are presently not possible.

Publications

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Harrison, N. and M. Jaime. Hidden valence transition in uranium ruthenium two silicon two. Submitted to *Nature Communications*. (LA-UR-19-21055)

Harrison, N. and P. H. Tobash. Resolution to the missing entropy at the delta - alpha volume collapse in Pu-Ga alloys. Submitted to *Physical Review*. (LA-UR-20-24241)

Joyce, J. J., K. S. Graham, J. Zhu, G. H. Lander, T. Durakiewicz, J. M. Wills, P. H. Tobash, E. D. Bauer, J. N. Mitchell and H. Choi. Competing Electronic Configurations for PuTe and New Insight on Plutonium Metal. Submitted to *Physical Review Letters*. (LA-UR-19-20178)

*Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Physical Review X*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

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*Tutchton, R. M., W. Chiu, R. C. Albers, G. Kotliar and J. Zhu. Electronic Correlation Induced Expansion of Fermi Pockets in delta-Plutonium. 2020. *Physical Review B*. **101** (24): 245156. (LA-UR-19-29904 DOI: 10.1103/PhysRevB.101.245156)

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Hernandez, S. C. and J. M. Wills. First Principles Investigation of the electronic and magnetic structure of Pu6Fe. Presented at *Pu Futures 2018*. (San Diego, California, United States, 2018-09-09 - 2018-09-09). (LA-UR-18-23453)

Maiorov, B. A., J. B. Betts, F. F. Balakirev and A. Migliori. Temperature dependent and Real Time Studies of Elastic Moduli of \xce\xb4-239Pu and alloys. Presented at

Plutonium Futures. (san diego, California, United States, 2018-09-09 - 2018-09-14). (LA-UR-18-25818)

Tobash, P. H., E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, S. Richmond, D. Wheeler and T. Albrecht-Schmitt. Progress on the Thermophysical Properties of Some Plutonium Alloys and Compounds. Presented at *Pu Futures 2018*. (San Diego, California, United States, 2018-09-09 - 2018-09-09). (LA-UR-18-23371)

Books/Chapters

Tobash, P. H. and S. Bobev. Chemical Bonding and Structural Relationships in Extended Solids. (LA-UR-18-28530)

Reports

Nelson, C. A. Uncovering the role of 5f-electron magnetism in plutonium using capacitive dilatometry. Unpublished report. (LA-UR-19-20411)

Presentation Slides

Harrison, N. Magnetostriction of delta-plutonium. Presented at *Plutonium futures*, san diego, California, United States, 2018-09-09 - 2018-09-09. (LA-UR-18-28499)

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Harrison, N., P. H. Tobash, M. Jaime, S. Richmond, J. B. Betts and M. R. Wartenbe. Phase stabilization by electronic entropy in plutonium. Presented at *American Physical Society March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21885)

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Hernandez, S. C. Overview of using density functional theory for material science applications on Pu and its compounds. Presented at *Computational Data Science Approaches for Materials*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23136)

Hernandez, S. C. Density functional theory study of aging of Pu. . (LA-UR-20-21880)

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the Electronic and Magnetic Structure of Pu6Fe. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21830)

Kushwaha, S. K., M. K. Chan, N. Harrison, P. Ferrari Silveira Rosa, S. M. Thomas, E. D. Bauer, F. Ronning, J. Park and J. D. Thompson. Magnetic field induced Fermi liquid in a candidate topological Kondo insulator. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22244)

Maiorov, B. A., J. B. Betts, F. F. Balakirev, F. J. Freibert and A. Migliori. Temperature Dependent and Real Time Studies of Elastic Moduli of \xce\xb4-239Pu and Alloys. Presented at *Plutonium Futures*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-29991)

Migliori, A. and S. M. Ennaceur. Toward an understanding of aging in plutonium from direct measurements of stored energy. . (LA-UR-18-31769)

Tobash, P. H., E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, T. Albrecht-Schmitt and D. Wheeler. Thermophysical Property Studies on Pu Alloys and Compounds. Presented at *MRS 2018*, Phoneix, Arkansas, United States, 2018-04-02 - 2018-04-02. (LA-UR-18-22563)

Tobash, P. H., S. Richmond, E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, D. Wheeler and T. Albrecht-Schmitt. Progress on the Thermophysical Properties of Some Plutonium Alloys and Compounds. Presented at *Pu Futures 2018*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28267)

Tutchton, R. M. Correlation and Electron-phonon coupling in the Electronic structure of Plutonium. Presented at *Science in 3*, Los Alamos, New Mexico, United States, 2018-06-13 - 2018-06-13. (LA-UR-18-26227)

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Wartenbe, M. R., P. H. Tobash, N. Harrison, J. B. Betts, J. Singleton and L. E. W. Stritzinger. Plutonium in high magnetic fields. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22254)

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Hernandez, S. C. and J. M. Wills. First Principles Investigation of the Electronic and Magnetic Structure of Pu6Fe. Presented at *Pu Futures 2018*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28384)

Nelson, C. A., M. R. Wartenbe, S. M. Thomas, G. M. Schmiedeshoff, N. Harrison and P. H. Tobash. Assembling and Calibrating a Capacitive Dilatometer for Magnetostriction and Thermal Expansion Measurements. . (LA-UR-18-26970)

Richmond, S. Plutonium sample processing, grain growth and extraction by hydriding. . (LA-UR-19-21170)

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Tutchton, R. M. and J. Zhu. Temperature Dependent Phonon Dispersions of Non-magnetic delta-Plutonium. Presented at *Theory Frontiers in Actinide Sciences: Chemistry and Materials*, Santa Fe, New Mexico, United States, 2020-02-02 - 2020-02-05. (LA-UR-20-20745)

Rational Design of Halide Perovskites for Next Generation Gamma-ray Detection

Sergei Tretiak
20180026DR

Project Description

This project will address two key national security challenges: (i) we will establish the scientific understanding and the design principles for a new halide perovskite materials technology for the fabrication of radiation detectors, critical for several Los Alamos National Laboratory and NNSA missions; (ii) we will demonstrate a proof-of-concept room temperature (RT) operated gamma ray detector with sensitivity and energy resolution exceeding that of cadmium-zinc-telluride (CZT) detectors, which represent the state-of-the-art for RT Gamma-ray detection.

Publications

Journal Articles

*Appavoo, K., W. Nie, J. -. Blancon, J. Even, A. D. Mohite and M. Y. Sfeir. Ultrafast optical snapshots of hybrid perovskites reveal the origin of multiband electronic transitions. 2017. *Physical Review B*. **96** (19): 195308. (LA-UR-17-29873 DOI: 10.1103/PhysRevB.96.195308)

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Huang, H., H. Tsai, R. Raja, S. Lin, D. Ghosh, C. Hou, J. Shyue, C. Chang, S. Tretiak, W. Chen, W. Nie, K. Lin and L. Wang. Robust un-encapsulated perovskite solar cells protected by fluorinated fullerene electron transporting layer. Submitted to *Nature*. (LA-UR-20-23214)

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Jenen, K. L., A. Shabaev, S. G. Lambrakos, D. Finkenstadt, A. J. Neukirch, N. A. Moody, S. Tretiak, D. A. Shiffler and J. J. Petillo. Analytic Model of Electron Transport Through and Over Non-Linear Barriers. Submitted to *Journal of Applied Physics*. (LA-UR-20-22694)

Jensen, K. L., A. Shabaev, S. G. Lambrakos, D. Finkenstadt, J. J. Petillo, A. J. Neukirch, A. M. Alexander, J. M. Smedley, N. A. Moody, H. Yamaguchi, F. Liu and S. Tretiak. An Extended Moments Model of Quantum Efficiency for Metals and Semiconductors. Submitted to *New Journal of Physics*. (LA-UR-20-23027)

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Ruddlesden-Popper Lead Halide Perovskite Thin Films. Submitted to *ACS Nano*. (LA-UR-20-21239)

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Leveillee, J. A., C. Katan, J. Even, A. Mohite, S. Tretiak, A. Schleife and A. J. Neukirch. First principles survey of organic spacer candidates for tuned light emission from layered hybrid perovskite materials. Submitted to *ACS Energy Letters*. (LA-UR-19-20225)

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Driven Quantum Matter: A Route Towards Novel Phases

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20190026DR

Project Description

The discovery of new materials has played a significant part in nearly every technological leap forward. To date, these advances have relied on conventional materials, which are now reaching their intrinsic limits. Quantum materials can enable us to overcome this, as they offer a host of unique properties that could be the basis of the next technological revolution, impacting areas including quantum computing and energy-efficient sensing. However, it has been difficult to tailor them for such applications, likely because conventional equilibrium tuning methods (e.g., temperature and pressure) make it difficult to realize a desired state of matter. Intense, transient electromagnetic (EM) fields have recently emerged as an exciting alternative for driving quantum materials into new states. However, these states have thus far been discovered by chance, making it vital to develop new approaches for predicting and controlling EM-driven phases. The objective of this project is to move beyond serendipitous discovery to demonstrate a world-leading capability for predicting and realizing novel EM-driven quantum phases, accomplished by pursuing an integrated theoretical and experimental approach focusing on three representative classes of quantum materials. This will impact a wide range of mission-relevant objectives, including novel materials for energy-efficient sensing, data storage, and computation.

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Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials

Blas Uberuaga
20190043DR

Project Description

Testing of refurbished (aka Lifetime Extension), reused, or newly designed weapon components is central to the mission of the Enhanced Capabilities for Subcritical Experiments (ECSE) project. While the ECSE accelerator will produce an excellent x-ray sources that will be used for weapons radiography, a great deal of leverage (both in terms of cost and radiographic quality) comes from what happens in the radiographic imaging system. This project proposes to produce a new scintillator material, the most important component in the imaging system, that provides options to improve the performance of ECSE. Perhaps it goes without stating, but greater radiographic system performance for ECSE will vastly increase the value of the experiments performed there. Looking further afield, a deeper understanding of the important interplay between the atomic and condensed matter physics that determines scintillator performance will help us to improve these materials for other missions relevant to the National Nuclear Security Administration as well as Department of Energy writ large.

Publications

Journal Articles

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Liu, X., G. Pilania, A. A. Talapatra, C. R. Stanek and B. P. Uberuaga. Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. 2020. *ACS Applied Materials & Interfaces*. **12** (41): 46296-46305. (LA-UR-20-24907 DOI: 10.1021/acsami.0c13236)

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Sharma, V., P. Kumar, P. Dev and G. Pilania. Machine Learning Substitutional Defect Formation Energies in ABO3 Perovskites. Submitted to *Journal of Applied Physics*. (LA-UR-20-24008)

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Wang, Z., K. Anagnost, C. W. Barnes, D. M. Dattelbaum, E. R. Fossum, E. Lee, J. Liu, J. J. Ma, W. Z. Meijer, W. Nie, C. M. Sweeney, A. C. Therrien, H. Tsai and X. Yue. Billion-pixel X-ray camera (BiPC-X) for wide field-of-view measurements. Submitted to *Review of Scientific Instruments*. (LA-UR-21-20086)

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Smith, E., B. W. Wiggins and C. G. Richards. Developments in garnet based scintillating composites for radiation detection applications. Presented at *SPIE Optics*

+ Photonics. (San Diego, California, United States, 2020-08-23 - 2020-08-27). (LA-UR-20-25861)

Books/Chapters

Pilania, G., P. Balachandra, J. E. Gubernatis and T. Lookman. Data-Based Methods for Materials Design and Discovery Basic Ideas and General Methods. (LA-UR-19-31822)

Reports

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Pestovich, K. S., C. J. Chandler, J. H. Clayton, B. P. Uberuaga and K. J. Mcclellan. Scintillator Discovery & Development within (Y,Lu,Gd)3(Al,Ga)5O12:Ce. Presented at *Scintillation Materials Research Center Research Group Meeting*, Knoxville, Tennessee, United States, 2020-09-14 - 2020-09-14. (LA-UR-20-27011)

Pilania, G. Materials that Glow: Discovering and designing new scintillators with machine learning. Presented at *Artificial Intelligence for Materials Science (AIMS) at NIST*, Gaithersburg, Maryland, United States, 2019-08-01 - 2019-08-01. (LA-UR-19-28296)

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Williams, L., E. Kioupakis and G. Pilania. Machine Learning with Local Environment Descriptors to Predict New Scintillator Materials. Presented at *Michigan Institute for Computational Discovery in Engineering*, Ann Arbor, Michigan, United States, 2019-04-10 - 2019-04-10. (LA-UR-19-23018)

Proximity Effects at Meso-, Nano-, and Atomic Scales: A new Path to Quantum Functionalities

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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.

Publications

Journal Articles

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Zhu, J., G. Dhakal, M. M. Hosen, A. Ghosh, C. A. Lane, K. Gornica, M. J. Winiarski, K. Dimitri, F. Kabir, C. Sims, S. Regmi, W. D. Neff, D. Kaczorowski, T. Klimczuk and M. Neupane. Observation of topological surface state in a superconducting material. Submitted to *Physical Review Letters*. (LA-UR-19-31397)

Presentation Slides

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Posters

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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)

Control Of Microstructural Instabilities in Composites (COMIC): A Pathway to Realizing Damage Resistant Metals

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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.

Publications

Journal Articles

Chakraborty, A., A. Hunter and L. Capolungo. Effect of microstructure, layer thickness, and interface behavior on the plasticity of accumulative roll bonded nano-metallic laminates using dislocation dynamics simulations. Submitted to *Journal of Materials Research*. (LA-UR-20-30289)

Chen, J. and S. J. Fensin. Effect of Local Structure and Stoichiometry on the Dynamic Behavior of Bi-metal interfaces. Submitted to *Journal of Applied Physics*. (LA-UR-21-22436)

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Liu, X., L. Capolungo and A. Hunter. Screw dislocations impingement and slip transfer at fcc-bcc semicoherent interfaces. Submitted to *Scripta Materialia*. (LA-UR-21-20512)

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Zecevic, M., K. Bennett, D. J. Luscher and R. A. Lebensohn. New self-consistent homogenization for thermo-elastic polycrystals with imperfect interfaces. 2020. *Mechanics of Materials*. 103651. (LA-UR-20-24726 DOI: 10.1016/ j.mechmat.2020.103651)

Presentation Slides

Carpenter, J. S., D. R. Coughlin, R. J. Mccabe, C. Miller, T. J. Nizolek, C. M. J. Osborn and M. M. Schneider. Probing Differences in Processing and Texture in FCC/BCC Nanolaminates Fabricated via Accumulative Roll Bonding. Presented at *MS&T 2020*, Pittsburgh, Pennsylvania, United States, 2020-11-02 - 2020-11-02. (LA-UR-20-28102)

Chakraborty, A., A. Hunter and L. Capolungo. Capturing kinetics of FR sources using DD simulations. . (LA-UR-21-20738)

Chakraborty, A., M. Zecevic, X. Liu, A. Hunter, R. A. Lebensohn and L. Capolungo. Understanding plasticity in nano-metallic laminates using dislocation dynamics simulations. . (LA-UR-21-21588)

Mccabe, R. J., M. Zecevic, T. J. Nizolek, N. Li, M. M. Schneider, C. Miller, C. M. J. Osborn, D. R. Coughlin, R. A. Lebensohn and J. S. Carpenter. Texture evolution of individual layers during accumulative roll bonding of Fe/fcc metallic laminates. Presented at *MS&T20 Virtual*, Los Alamos, New Mexico, United States, 2020-11-02 - 2020-11-06. (LA-UR-20-28399)

Mccabe, R. J., M. Zecevic, Y. Zhang, N. Li, J. G. Gigax, T. J. Nizolek and J. S. Carpenter. Layer dependent plasticity in accumulative roll bonded FCC/BCC metallic laminates. Presented at *TMS 2021Annual Meeting & Exhibition*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21826)

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Zecevic, M., R. A. Lebensohn, K. Bennett and D. J. Luscher. Analytical and computational homogenization of heterogeneous microstructures with imperfect interfaces. Presented at *14th World Congress in Computational Mechanics*, Paris, France, 2021-01-11 - 2021-01-15. (LA-UR-20-29723)

Zecevic, M., R. A. Lebensohn, T. J. Nizolek, R. J. Mccabe and L. Capolungo. FFT-based modeling of strain localization in nano-metallic laminates. Presented at *TMS 2021 (virtual conference)*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21750)

Zhang, Y., Q. Li, M. Gong, T. Niu, S. Xue, J. Wang, H. Wang, X. Zhang and N. A. Richter. Deformation behavior and phase transformation of nanotwinned Al/Ti multilayers. Presented at *TMS 2021 Virtual Annual Meeting*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21787)

Quantum Photonics with Semiconductor Nanocrystals

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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.

Publications

Journal Articles

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Reports

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Boom or Bust? Predicting Explosive Safety under Impacts

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20180100DR

Project Description

High explosives are a component of conventional and nuclear weapons. We seek to understand the fundamental origins of the impact safety of explosives over a wide range of loading rates. Impacts on explosives generate localized deformation and fracture which can lead to ignition. Our ability to accurately predict how deformation occurs has been limited both by the complexity of these materials and the challenges of interrogating the structural responses of these materials under violent loading. We have made huge strides toward overcoming both of these obstacles in recent years. First, in situ, time-resolved x-ray imaging and diffraction at the Advanced Photon Source have provided new insights into how materials deform. Developments in theory and simulation have led to truly predictive models of explosives responses under shock loading. Moreover, the coupling between deformation and temperature can now be measured directly with vibrational spectroscopy. We will greatly extend our proof-of-concept work so we can understand and predict the impact responses and hence safety of cyclotrimethylene trinitramine (RDX) and cyclotetramethylene tetranitramine (HMX) single crystals and composites, two explosives of importance to DOD and DOE. Finally, we will apply our modeling framework to computationally design new energetic materials with microstructures tailored for impact safety.

Technical Outcomes

The final product of this project was an experimentally validated predictive capability for how energetic materials respond to impacts at the crystal, defect, and composite scales that control safety. This coordinated experimental-theory research effort has enabled an entirely new generation of microstructure aware models, built on a framework of realistic underlying sub-scale physics that was substantially less well-known before this project (i.e. especially for inclusion of the effects of anisotropy).

Publications

Journal Articles

Addessio, F. L., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Investigation of Plate Impact Experiments on Single-Crystal RDX Above the Phase Transformation Pressure. Submitted to *Journal of Applied Physics*. (LA-UR-20-22056)

Addessio, F. L., N. Mohan, D. J. Luscher, B. M. Morrow, M. J. Cawkwell, C. Liu, C. Meredith and K. J. Ramos. A Single-Crystal Model for the Deformation of Cyclotrimethylene Trinitramine including Plastic Slip, Crack Growth and Crack Friction. Submitted to *Journal of Applied Physics*. (LA-UR-20-21101)

Cawkwell, M. J., M. Zecevic, D. J. Luscher and K. J. Ramos. Complete equations of state for cyclotetramethylene tetranitramine. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-20-27725)

Cawkwell, M. J., N. Mohan, D. J. Luscher and K. J. Ramos. Dissociation of <111> dislocations on {1-10} in pentaerythritol tetranitrate. Submitted to *\tPhilosophical Magazine* . (LA-UR-18-27828)

Lazarz, J. D., C. A. Bolme, K. J. Ramos and S. D. Jacobsen. Optical crystallography of acetaminophen and assessment of structure-property effects of impurities by refractometry. Submitted to *International Journal of Pharmaceutics*. (LA-UR-18-28787)

Lazarz, J. D., S. D. Jacobsen, P. Dera, Y. Hu, Y. Meng and C. R. Bina. High-pressure phase transitions of clinoenstatite. Submitted to *American Mineralogist*. (LA-UR-18-26664)

Lazarz, J. D., S. D. Mcgrane, R. T. Perriot, C. A. Bolme and K. J. Ramos. Anisotropic Thermal Conductivity and Elasticity of RDX Using Impulsive Stimulated Thermal Scattering. Submitted to *AIP Conference Proceedings*. (LA-UR-19-27498)

*Luscher, D. J., M. A. Buechler, D. J. Walters, C. A. Bolme and K. J. Ramo. On computing the evolution of temperature for materials under dynamic loading. 2018. *International Journal of Plasticity*. **111**: 188-210. (LA-UR-18-21769 DOI: 10.1016/j.ijplas.2018.07.014)

*Luscher, D. J., M. J. Cawkwell, K. J. Ramos, R. L. Sandberg and C. A. Bolme. Interpreting Experimental Results from Shock Impacts on Single Crystal PETN in the Context of Continuum Models. 2020. *Propellants, Explosives, Pyrotechnics*. **45** (2): 284-294. (LA-UR-19-26192 DOI: 10.1002/prep.201900228)

*Luscher, D. J., M. J. Cawkwell, K. J. Ramos, R. L. Sandberg and C. A. Bolme. Interpreting Experimental Results from Shock Impacts on Single Crystal PETN in the Context of Continuum Models. 2020. *Propellants, Explosives, Pyrotechnics*. **45** (2): 284-294. (LA-UR-19-26299 DOI: 10.1002/prep.201900228)

Mohan, N., D. J. Luscher, M. J. Cawkwell, F. L. Addessio and K. J. Ramos. Modeling Microstructural Effects on Heterogeneous Temperature Fields within Polycrystalline Explosives. 2021. *Propellants, Explosives, Pyrotechnics*. prep.202000282. (LA-UR-20-27778 DOI: 10.1002/prep.202000282)

Mohan, N., M. J. Cawkwell, F. L. Addessio, K. J. Ramos and D. J. Luscher. Modeling microstructural effects on heterogeneous temperature fields within polycrystalline explosives. Submitted to *Journal of Applied Physics*. (LA-UR-19-29280)

Powell, M. S., D. S. Moore, S. F. Son and S. D. Mcgrane. Shocked TNT Paper V4. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-20-27621)

Zecevic, M., F. L. Addessio, M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Single Crystal Plasticity Model with Deformation Twinning for the High Rate Deformation of \xce\xb2-HMX. Submitted to *AIP Conference Proceedings*. (LA-UR-19-26875)

*Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. An implementation of the phase-field model based on coupled thermomechanical finite element solvers for large-strain twinning, explicit dynamic fracture and the classical Stefan problem. 2020. *Modelling and Simulation in Materials Science and Engineering*. **28** (5): 055002. (LA-UR-19-29290 DOI: 10.1088/1361-651X/ab8357)

Conference Papers

Walters, D. J., K. J. Ramos, F. L. Addessio, C. E. Armenta, J. L. Barber, C. A. Bolme, M. J. Cawkwell, L. Dresselhaus-Cooper, A. E. Gleason Holbrook, A. C. Golder, E. L. Hartline, B. J. Jensen, H. J. Lee, D. J. Luscher, C. S. Meredith, I. Nam, T. H. Pierce, C. Pulham, P. Rigg, R. L. Sandberg, M. Seaberg, N. Sinclair and G. K. Windler. Mesoscale Mechanics of Energetic Materials: A Coordinated Experiment-theory Effort Using New In Situ Probes. Presented at *16th International Detonation Symposium*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-20). (LA-UR-18-25734)

Reports

Liu, C. and C. M. Cady. Observation of Cracking and Measurement of Fracture Toughness in Brittle/Quasi-Brittle Solids. Unpublished report. (LA-UR-20-28805)

Mohan, N., M. J. Cawkwell, F. L. Addessio, K. J. Ramos and D. J. Luscher. Characterizing Grain-Size Effects in the Shock Heating of Idealized PBXs. Unpublished report. (LA-UR-19-28308)

Mohan, N., M. J. Cawkwell, F. L. Addessio, K. J. Ramos and D. J. Luscher. Characterizing Grain-Size Effects in the Shock Heating of Idealized PBXs. Unpublished report. (LA-UR-19-28307)

Perriot, R. T., M. S. Powell, J. D. Lazarz, C. A. Bolme, D. S. Moore, S. D. Mcgrane, M. J. Cawkwell and K. J. Ramos. Pressure, temperature, and orientation dependent thermal conductivity of \xce\xb1-1,3,5-trinitro-1,3,5-triazinane (\xce\xb1-RDX). Unpublished report. (LA-UR-21-22762)

Presentation Slides

Addessio, F. L., M. J. Cawkwell, C. Liu, D. J. Luscher, C. Meredith, N. Mohan, B. M. Morrow and K. J. Ramos. Analysis of Plate Impact and Hopkinson Bar Experiments for Single-Crystals of RDx. Presented at *APS Shock Compression of Condensed Matter Meeting*, Portland, Oregon, United States, 2019-06-17 - 2019-06-21. (LA-UR-19-25257)

Addessio, F. L., N. Mohan, D. J. Luscher, M. J. Cawkwell and K. J. Ramos. Theory and Model Development for Single-Crystals of RDX: Phase Transformations through Damage. Presented at *LANL workshop on predicting HE safety under impacts*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-21. (LA-UR-19-21305)

Cady, C. M. and C. Liu. Quantitative Investigation of Fracture in Brittle/Quasi-Brittle Solids. Presented at *Materials Science & Technology 2019*, Portland, Oregon, United States, 2019-09-29 - 2019-10-03. (LA-UR-19-29593)

Cawkwell, M. J. Large-scale Accelerated Quantum Molecular Dynamics (w17_latteqmd). . (LA-UR-19-21928)

Cawkwell, M. J., F. L. Addessio, D. J. Luscher, J. L. Barber and K. J. Ramos. Mechanical Properties of Energetic Materials Under Impact at the Single Crystal and Mesoscales. Presented at *2018 Mach Conference*, Annapolis, Maryland, United States, 2018-04-04 - 2018-04-06. (LA-UR-18-22679)

Cawkwell, M. J., K. J. Ramos, C. Liu, F. L. Addessio, D. J. Luscher, S. D. Mcgrane, D. Montgomery, N. Mohan, M. Zecevic, J. D. Lazarz, D. S. Moore, R. T. Perriot and C. M. Cady. LDRD-DR 20180100 Review: Boom or Bust? Predicting Explosive Safety Under Impact. Presented at *Workshop on Predicting Explosive Safety Under Impacts*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-21. (LA-UR-19-21635)

Cawkwell, M. J., N. Mohan, D. J. Luscher, R. T. Perriot and K. J. Ramos. Atomic-scale Simulations of Explosives: Applications to EOS, thermal transport, surface energies, and crystal plasticity. Presented at *LANL workshop on predicting HE safety under impacts*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-21. (LA-UR-19-21233)

Cawkwell, M. J., S. D. Mcgrane, K. J. Ramos and D. J. Luscher. Modeling explosives at the mesoscale: areas for collaboration. Presented at *AFOSR MURI Kick-Off Meeting*, Niceville, Florida, United States, 2019-09-19 - 2019-09-19. (LA-UR-19-29310)

Lazarz, J. D., S. D. Mcgrane, R. T. Perriot, C. A. Bolme, M. J. Cawkwell and K. J. Ramos. Anisotropic Thermal Conductivity and Elasticity of RDX Using Impulsive Stimulated Thermal Scattering. Presented at *APS March Meeting*, denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21850)

Lazarz, J. D., S. D. Mcgrane, R. T. Perriot, D. S. Moore, C. A. Bolme and K. J. Ramos. Anisotropic Thermal Conductivity and Elasticity of RDX Using Impulsive Stimulated Thermal Scattering Experimentally Solving the Heat Equation. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25188)

Lazarz, J. D., S. D. Mcgrane, R. T. Perriot and D. S. Moore. Experimentally solving the heat equation impulsively stimulated light scattering and stokes/anti-stokes Raman. Presented at *LANL CHE Grand Challenge Technical Symposium*, Los Alamos, New Mexico, United States, 2019-05-21 - 2019-05-22. (LA-UR-19-24623)

Liu, C. Fracture in PBX 9502 High Explosive: Effect of Loading Rate & Material Orientation. . (LA-UR-17-30625)

Liu, C., C. M. Cady, K. J. Ramos, B. M. Morrow and C. Meredith. Dynamic Compression of RDX Single Crystal and High Explosives. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21272)

Liu, C., C. M. Cady and K. J. Ramos. Experimental Investigation of Cracking and Fracture in Brittle/Quasi-Brittle Materials Using DIC. Presented at *LDRD-DR review*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-21. (LA-UR-19-21148)

Liu, C., C. M. Cady and R. R. Stevens. Observation of Cracking and Measurement of Fracture Toughness in Graphite. Presented at *2018 ASME International Mechanical Engineering Congress and Exposition (IMECE)*, Pittsburgh, Pennsylvania, United States, 2018-11-11 - 2018-11-15. (LA-UR-18-30640)

Liu, C., C. Meredith, B. M. Morrow, C. M. Cady and K. J. Ramos. Dynamic Deformation of RDX Single Crystal Using Miniature SHPB and High-Speed Photography. Presented at *2019 Society of Experimental Mechanics (SEM) Annual Conference & Exposition on Experimental and Applied Mechanics*, Reno, Nevada, United States, 2019-06-03 - 2019-06-06. (LA-UR-19-24988)

Luscher, D. J., N. Mohan, M. Zecevic, F. L. Addessio, M. J. Cawkwell and K. J. Ramos. Continuum modeling of the mesoscale response of single-crystal and polycrystalline explosive materials. Presented at *LDRD-DR 20180100 First-Year Review*, Los Alamos, New Mexico, United States, 2019-02-21 - 2019-02-21. (LA-UR-19-21566)

Mcgrane, S. D. Stokes/anti-Stokes Raman scattering for temperature measurement in explosives. . (LA-UR-18-24969)

Mcgrane, S. D. Experimentally solving the heat equation with Impulsively Stimulated Light Scattering and Stokes/anti-Stokes Raman. . (LA-UR-19-21343)

Mohan, N. Damage Mechanics Interview. . (LA-UR-19-26847)

Mohan, N., D. J. Luscher, M. J. Cawkwell, F. L. Addessio and K. J. Ramos. Temperature evolution in polycrystalline PBX under impacts. Presented at *APS March Meeting*, boston, Massachusetts, United States, 2019-03-02 - 2019-03-08. (LA-UR-19-21641)

Mohan, N., D. J. Luscher, M. J. Cawkwell, F. L. Addessio and K. J. Ramos. Grain-size effects in the shock heating of idealized PBXs. Presented at *APS GSCCM*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25409)

Mohan, N., M. J. Cawkwell, D. J. Luscher, K. J. Ramos and F. L. Addessio. Anisotropic Damage Model for RDX under Impact. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21535)

Montgomery, D. Quantitative Phase Retrieval for Dynamic Compression Experiments. Presented at *Data Science & Computation for Dynamic Compression Experiments, Virtual Workshop*, Los Alamos, New Mexico, United States, 2020-09-08 - 2020-09-11. (LA-UR-20-26982)

Morrow, B. M., F. L. Addessio, C. A. Bronkhorst, E. K. Cerreta, B. Feng, D. R. Jones, R. A. Lebensohn, C. Liu and K. J. Ramos. An Experimental Perspective on Computational Validation for Dynamic Mechanical Behavior. Presented at *MS&T 2019*, Portland, Oregon, United States, 2019-09-29 - 2019-09-29. (LA-UR-19-29675)

Morrow, B. M., F. L. Addessio, C. S. Meredith, K. J. Ramos, C. Liu and C. M. Cady. Experiments & Modeling to Explore Dynamic Behavior of Materials via Kolsky Bar at Equilibrium & Beyond. Presented at *TMS Annual Meeting 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-21351)

Perriot, R. T., M. J. Cawkwell, J. D. Lazarz, S. D. Mcgrane and K. J. Ramos. Temperature, pressure, and orientation dependence of the thermal conductivity of \xf0\x9d\x9c \xb6- and \xf0\x9d\x9c\xb8-RDX. Presented at *APS-SCCM 2019*, Portland, Oklahoma, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25602)

Ramos, K. J. In Situ Investigation of Phase Transformation in Cyclotrimethylene Trinitramine (RDX) During Shock Loading Using X-ray Diffraction. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK19)*, Portland, Oregon, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25457)

Ramos, K. J. and M. J. Cawkwell. Mesoscale Mechanics of Energetic Materials: A Coordinated Experiment-Theory Effort Using New In Situ Probes. . (LA-UR-18-26515)

Zecevic, M., F. L. Addessio, M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Single crystal plasticity model with deformation twinning for the high rate deformation of \xce\xb2-HMX. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK19)*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25251)

Posters

Lazarz, J. D., S. D. Mcgrane, B. M. Morrow, C. M. Cady, C. Liu, C. S. Meredith, D. T. Casem and K. J. Ramos. Split Hopkinson Pressure Bar (SHPB) Diagnostics: Overview and Integration. . (LA-UR-19-21247)

Lazarz, J. D., S. D. Mcgrane, R. T. Perriot, C. A. Bolme and K. J. Ramos. Anisotropic Thermal Conductivity and Elasticity of RDX Using Impulsive Stimulated Thermal Scattering. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25192)

Lazarz, J. D., T. J. Nizolek and K. J. Ramos. Orientation Imaging Microscopy Using Polarized Light. . (LA-UR-19-21248)

Mohan, N., D. J. Luscher, M. J. Cawkwell, F. L. Addessio and K. J. Ramos. Temperature distributions from Finite Element Modeling of polycrystalline PBX under Shock Loading. . (LA-UR-19-21295)

Mohan, N., M. J. Cawkwell, F. L. Addessio, K. J. Ramos and D. J. Luscher. Grain-size effects in the shock heating of idealized PBXs. Presented at *2019 Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-09. (LA-UR-19-27860)

Morrow, B. M., C. E. Armenta and K. J. Ramos. Electron Microscopy for Characterization and Miniature DIC Patterning. Presented at *LDRD-DR Midterm Review*, Los Alamos, New Mexico, United States, 2019-02-19 - 2019-02-19. (LA-UR-19-21154)

Perriot, R. T. and M. J. Cawkwell. Temperature, Pressure, and Orientation Dependent Thermal Conductivity of \xf0\x9d\x9c\xb6- and \xf0\x9d\x9c\xb8-RDX from Atomistic Simulations. . (LA-UR-19-21221)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Single Crystal Plasticity Model with Deformation Twinning for the High Rate Deformation of \xf0\x9d\x9c\xb7-HMX. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-09. (LA-UR-19-27586)

Utilizing Crystalline Sponges to Perform Single Crystal X-ray Determination on Trace Amounts of Actinium Compounds

Brian Scott
20180128ER

Project Description

Actinium shows great promise as a cancer radioimmunotherapy agent. However, its scarcity has hindered chemical structure characterization with X-rays. Chemical structure is vital to understanding how actinium will behave in biological systems and also for designing therapeutic agents. This work will develop techniques to perform X-ray single crystal characterization using trace amounts of actinium absorbed into porous crystals. These porous crystals, known as metal-organic-frameworks (MOF's), are composed of metal centers linked together with organic molecules to form a three-dimensional structure with open pores. Microgram quantites of actinium are not sufficient to grow crystals for X-ray studies, but do provide ample material for an actinium-MOF crystal that can be used for X-ray structure determination. An MOF crystal large enough for X-ray studies can absorb micrograms of actinium into its pores. An X-ray crystal structure of the actinium containing MOF crystal will yield the structure of the MOF and the absorbed actinium species. Besides informing radioimmunotherapy development using actinium, this technique could also be used to determine chemical structure of trace amounts of chemical weapons agents, explosives, and other actinides and molecules of importance to national security.

Publications

Journal Articles

Klamm, B. E., T. E. Albrecht-Schmitt, R. E. Baumbach, B. S. Billow, F. D. White, S. A. Kozimor, B. L. Scott and A. M. Tondreau. Using Intrinsic Lewis-Acidity in the Generation of Bimetallic Lanthanide Complexes. Submitted to *Inorganic Chemistry*. (LA-UR-20-21131)

Books/Chapters

J. White, F. D. and M. L. Marsh. Recent Advances in Non-aqueous Transuranic Chemistry. (LA-UR-19-23811)

Reports

Scott, B. L., G. S. Goff, D. A. Yarotski, P. C. Dowden, L. E. Wolfsberg and G. Rodriguez. Experimental Signatures for Dynamic Plutonium Hydriding. Unpublished report. (LA-UR-19-20942)

Presentation Slides

Elkin, T. Development of novel MOFs for (CWA) emerging threats. Presented at *IMS Rapid response workshop*, Evanston, Illinois, United States, 2019-09-10 - 2019-09-12. (LA-UR-19-29055)

Root, H. D. Applications of Porphyrinoid Macrocycles in Molecular Sensing and f-Element Coordination. . (LA-UR-20-24682)

Electronic Structure of Putative Topological Kondo Insulators

Mun Chan
20180137ER

Project Description

We will develop the capability to study electronic and magnetic properties of materials under simultaneous ultra-high pressures and high-magnetic fields. This will be applied to the study of topologically correlated electron materials, a field that promises significant technological implications, including ultra-fast quantum computation and spintronics. It is of vital importance to the Los Alamos mission to understand the properties of materials under pressure. Crystalline properties are routinely tracked with x-rays. Our new experimental capability will allow for a determination of the electronic properties. This will foster new collaborations at the high-magnetic field laboratory at the Laboratory.

Publications

Journal Articles

Chan, M. K., T. Sarkar, J. Higgins, P. Mandal, N. Poniatowski and R. Greene. Strange Metallic Transport in the Antiferromagnetic Regime of Electron Doped Cuprates. Submitted to *Physical Review X*. (LA-UR-20-24641)

*Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Physical Review X*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

Visualizing Nanoscale Spatio-Temporal Dynamics in Single Quantum Systems

Peter Goodwin
20180189ER

Project Description

This project is responsive to the Laboratory mission in the Materials for the Future Focus area in that it strives, through the development of novel characterization methods for the visualization of excited state dynamics in nanoengineered structures, for 'linking across length and time scales … to achieve a multi-scale understanding, and ultimately control, of materials structure, dynamics and function.' These studies will uncover detailed aspects of quantum dot (QD) interparticle interactions that will be relevant toward designing and improving QD optoelectronic devices, displays, solar cells, biological labels, and other technologies, and will enable the discovery of new properties and unanticipated applications and devices involving QDs. These studies will also reveal features of electronic energy interactions unique to QDs and other nanoparticles, as well as features common to molecular systems in which excited state electronic interactions are important, such as organic molecule Förster resonance energy transfer (FRET), conjugated polymers, and biological photosynthetic complexes. Finally, this research will introduce new experimental methods and capabilities that can be exploited to investigate a wide variety of molecular and nanoscale systems, in which multiple emitters cluster, aggregate, or associate to transport electronic energy in a manner that is greater than the sum of its parts.

Publications

Journal Articles

*Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. Van Orden. Super-resolution photoluminescence lifetime and intensity mapping of interacting CdSe/CdS quantum dots. 2020. *Applied Physics Letters*. **116** (2): 021103. (LA-UR-19-30441 DOI: 10.1063/1.5132563)

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. Van Orden. Single Molecule Localization With Four Avalanche Photodiode Detectors. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-20171)

Ryan, D. P., M. K. Dunlap, S. Majumder, C. J. Sheehan, J. H. Werner, J. A. Hollingsworth, M. P. Gelfand and A. K. Van Orden. Dual-color super-resolution imaging for FRET measurements: Energy transfer among donor/acceptor pairs of quantum dots. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-20052)

*Ryan, D. P., M. K. Dunlap, S. Majumder, J. H. Werner, J. A. Hollingsworth, M. P. Gelfand, A. Van Orden and P. M. Goodwin. A framework for quantitative analysis of spectral data in two channels. 2020. *Applied Physics Letters*. **117** (2): 024101. (LA-UR-20-23550 DOI: 10.1063/5.0013998)

*Ryan, D. P., P. M. Goodwin, C. J. Sheehan, K. J. Whitcomb, M. P. Gelfand and A. Van Orden. Mapping Emission from Clusters of CdSe/ZnS Nanoparticles. 2018. *The Journal of Physical Chemistry C*. **122** (7): 4046-4053. (LA-UR-18-20821 DOI: 10.1021/acs.jpcc.7b10924)

Ryan, D. P., P. M. Goodwin, J. H. Werner, M. K. Dunlap, A. K. Van Orden and M. P. Gelfand. From Noise to Harmony: Calibration Methods for Electron Multiplying CCD Cameras. Submitted to *Optics Express*. (LA-UR-20-27551)

Presentation Slides

Dunlap, M. K. Time-resolved Super-resolution Microscopy Studies of Quantum Dot Aggregates. . (LA-UR-21-20441)

Dunlap, M. K. Time-Resolved Super-Resolution Microscopy Studies of Quantum Dot Clusters. . (LA-UR-21-21336)

Dunlap, M. K. Time-resolved super-resolution microscopy studies of quantum dot clusters. . (LA-UR-21-22308)

Goodwin, P. M., J. H. Werner, J. A. Hollingsworth, M. K. Dunlap, D. P. Ryan, S. Majumder, A. Van Orden and M. P. Gelfand. 20180189ER Visualizing Nanoscale Spatio-Temporal Dynamics in Single Quantum Systems. . (LA-UR-20-23772)

Ryan, D. P. Energy Flow through Quantum Dot Networks. . (LA-UR-18-25130)

Ryan, D. P., A. K. Van Orden, J. A. Hollingsworth, M. K. Dunlap, J. H. Werner, P. M. Goodwin, C. J. Sheehan, S. Majumder and M. P. Gelfand. Camera-based single-particle orientation imaging of quantum dots. Presented

at *SPIE Photonics West: BiOS*, San Francisco, California, United States, 2021-03-06 - 2021-03-11. (LA-UR-21-21334)

Ryan, D. P., M. K. Dunlap, P. M. Goodwin, J. H. Werner, J. A. Hollingsworth, S. Majumder, C. J. Sheehan, A. K. Van Orden and M. Gelfand. Dual-color Super-resolution Imaging of Quantum Dot Clusters. Presented at *SPIE Photonic West 2020*, San Francisco, California, United States, 2020-01-31 - 2020-02-06. (LA-UR-20-20728)

Ryan, D. P., M. K. Dunlap, S. Majumder, C. J. Sheehan, J. A. Hollingsworth, M. P. Gelfand, P. M. Goodwin and A. K. Van Orden. Super-resolution Imaging for Energy Transfer: Collective behavior from interacting quantum dots. Presented at *American Chemical Society Annual Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22627)

Ryan, D. P., P. M. Goodwin, J. H. Werner, C. J. Sheehan, J. A. Hollingsworth, S. Majumder, M. K. Dunlap, A. Van Orden and M. Gelfand. Energy Transfer Through Networks of CdSe/CdS Nanoparticles. Presented at *Gordon Research Conference on Colloidal Semiconductor Nanocrystals*, Smithfield, Rhode Island, United States, 2018-07-15 - 2018-07-20. (LA-UR-18-26595)

Posters

Abdollah-nia, F., M. K. Dunlap, J. Gann, D. P. Ryan, P. M. Goodwin, J. A. Hollingsworth, Y. Chen, J. S. Martinez, M. Gelfand and A. Van Orden. Single Molecule Experiments in the Van Orden Resarch Group. Presented at *Colorado State University Chemistry Graduate Student Recruiting Weekend*, Fort Collins, Colorado, United States, 2019-02-15 - 2019-02-15. (LA-UR-19-21376)

Dunlap, M. K., A. K. Van Orden and J. Gahn. Single Molecule Studies in the Van Orden Group. . (LA-UR-21-21337)

Dunlap, M. K., D. P. Ryan, J. H. Werner, J. A. Hollingsworth, M. Gelfand, A. Van Orden and P. M. Goodwin. A Lifetime Imaging Super-Resolution Microscope. Presented at *ACS Spring 2019 National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-03. (LA-UR-19-23084)

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, J. A. Hollingsworth, M. Gelfand and A. Van Orden. Sub-Nanosecond Superresolution Imaging of Energy Transfer in CdSe/CdS Quantum Dot Clusters. . (LA-UR-19-24114)

Dunlap, M., D. P. Ryan, M. Gelfand and P. M. Goodwin. Quantum Dot Localization with Time Resolved Super-Resolution Tracking Microscopy. Presented at *Annual Meeting of the APS Four Corners Section*, Fort Collins, New Mexico, United States, 2017-10-20 - 2017-10-21. (LA-UR-17-29934)

Dunlap, M., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. K. Van Orden. Characterizing the Spatial Information of a Superresolution Fluorescence Lifetime Imaging Microscope. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28791)

Ryan, D. P., M. Dunlap, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand, A. K. Van Orden and C. J. Sheehan. Energy Transfer Through Networks of CdSe/CdS Nanoparticles. Presented at *Gordon Research Conference on Colloidal Semiconductor Nanocrystals*, Smithfield, Rhode Island, United States, 2018-07-14 - 2018-07-20. (LA-UR-18-25908)

Ryan, D. P., S. Majumder, J. A. Hollingsworth, J. H. Werner, P. M. Goodwin, A. K. Van Orden, M. K. Dunlap and M. P. Gelfand. Emission Dynamics from Clusters of Quantum Dots. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29347)

Ryan, D. P., S. Majumder, J. A. Hollingsworth, P. M. Goodwin, J. H. Werner, M. K. Dunlap, A. K. Van Orden and M. P. Gelfand. Super-resolution Orientation Imaging: A Microscopy Method for Measuring Structure in Biological Samples. Presented at *Biophysical Society Meeting*, San Francisco, California, United States, 2020-02-14 - 2020-02-19. (LA-UR-20-21373)

Improved Biologically Friendly Polymer Drag Reducers From Novel Architectures

Paul Welch
20180220ER

Project Description

The research described in this proposal will directly address the Objective Capability Area of Mitigating Impacts of Global Energy Demand Growth called out in the Los Alamos Energy Security Strategy. Specifically, we will address the objective of "Integrating multi-scale measurements, modeling,and uncertainty quantification to validate predictions to support decisions and investments in energy systems with a goal of anticipating risks, disruptions, impacts, and consequences." This project will produce a series of polymers designed to reduce drag in aqueous flows. The project will study the molecular physics involved in the polymer interactions in turbulent environments over a range of length and time scales using a novel combination of experimental and modeling techniques. Success in this project will produce new insight into the importance of molecular architecture in drag reduction, facilitating the design of new materials. In particular, we will learn: 1) whether intrinsically multi-time scale materials perform better in typical drag reduction applications; 2) how best to design the distribution of molecular time scales to optimally impact realistic flow fields; and 3) the biologically friendly chemical architectures that most likely satisfy that distribution.

Publications

Journal Articles

J. Welch, P. M. and C. F. Welch. Calculating Dendrimer Titration Curves through Quantum Annealing. Submitted to *ACS Macro Letters*. (LA-UR-19-27637)

Posters

Schmidt, J. G., C. Schein, D. Beasley, M. Braun and D. Weaver. Stabilized PCP-Consensus Peptides for Flavi- and Alphavirus Vaccines and Therapies. Presented at *CBS&T*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-30920)

Ultrafast X-ray Imaging Using Slow, Visible Cameras

Pamela Bowlan
20180242ER

Project Description

New bright sources of femtosecond (10-15 seconds) X-ray pulses are revolutionizing materials science giving atomic-scale snap shots of how materials behave in extreme conditions like high pressure or temperature. A major impediment in these experiments are the detectors which have temporal resolutions up to six orders of magnitude slower than the X-ray pulses, smearing out the dynamics being studied, and making it challenging to even diagnose the X-ray source. Future X-ray Free Electron Lasers, aimed to directly address DOE/NNSA mission goals like manufacturing science or dynamics in explosives, will use even higher X-ray photon energies and operate at higher X-ray pulse frequencies, for which no detector exists. Our work offers a novel, potentially transformative solution, where interacting an X-ray and visible light pulse in the right medium encodes the X-ray pulse's spatial and temporal information (i.e., the X-ray image and its femtosecond temporal evolution) in the visible light, making it possible to measure femtosecond time resolved X-ray images with standard visible cameras. This technology will both improve the capabilities at current DOE X-ray sources, and also help to motivate and build new sources optimized specifically for NNSA mission-relevant applications.

Publications

Journal Articles

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Measuring an ultrashort pulse in a slowly responding, absorbing medium. Submitted to *Optics Express*. (LA-UR-20-30027)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Response Letter. Submitted to *Optics Express*. (LA-UR-21-21553)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Supplemental Information for Measuring an ultrashort, ultraviolet pulse in a slowly responding, absorbing medium. Submitted to *Optics Express*. (LA-UR-21-21552)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Measuring an ultrashort, ultraviolet pulse in a slowly responding, absorbing medium. Submitted to *Optics Express*. (LA-UR-21-21551)

Jones, T. N., W. K. Peters, A. V. Efimov, R. L. Sandberg, D. A. Yarotski, R. P. Trebino and P. R. Bowlan. Measuring an ultraviolet ultrashort pulse by encoding it in a near-infrared nonlinear-optical signal pulse. Submitted to *OSA Continuum*. (LA-UR-20-24221)

Jones, T. N., W. K. Peters, A. V. Efimov, R. L. Sandberg, D. A. Yarotski, R. P. Trebino and P. R. Bowlan. Encoding the complete electric field of an ultraviolet ultrashort laser pulse in a near-infrared nonlinear-optical signal. Submitted to *Optics Express*. (LA-UR-20-26396)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, R. Trebino, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. All-optical single shot complete electric field measurement of extreme ultraviolet free electron laser pulses. Submitted to *Nature Photonics*. (LA-UR-20-27156)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, R. Trebino, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. All-optical single shot complete electric field measurement of extreme ultraviolet free electron laser pulses. Submitted to *Optica*. (LA-UR-21-20565)

Trebino, R., R. Jafari, S. Akturk, P. Piksarv, P. R. Bowlan, H. Valtna-Lukner, P. Saari, Z. Guang, P. Zhu and G. Steinmeyer. Tutorial: The Measurement of Ultrashort Laser Pulses. Submitted to *Journal of Applied Physics*. (LA-UR-20-24953)

Reports

Bowlan, P. R. Ultrafast Control of Material Properties though Core Electrons. Unpublished report. (LA-UR-18-21644)

Presentation Slides

Bowlan, P. R., M. S. Powell and S. D. Mcgrane. Ultrafast mid-IR measurements during shock. Presented at *Shocked chemistry LDRD review*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-06. (LA-UR-18-20743)

Bowlan, P. R., T. N. Jones and R. L. Sandberg. Travis' LANL Experience. Presented at *Meeting with Rick Trebino's*

research group (talk to be given by Travis Jones), Atlanta, Georgia, United States, 2019-01-15 - 2019-01-15. (LA-UR-19-20252)

Jones, T. N. Complete Temporal Measurement of Low-Intensity and High-Frequency Ultrashort-Presentation. . (LA-UR-20-29379)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. L. Sandberg, R. Trebino and P. R. Bowlan. Measuring ultraviolet, femtosecond pulses in a medium with a slow response. Presented at *Conference on Lasers and Electro-Optics (CLEO)*, San Jose, California, United States, 2020-05-10 - 2020-05-15. (LA-UR-20-23467)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, R. Trebino, R. L. Sandberg, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. Single-shot Measurement of Extreme Ultraviolet Free Electron Laser Pulses. Presented at *Conference on Lasers and Electro-optics*, San Joase, California, United States, 2020-05-11 - 2020-05-11. (LA-UR-20-23468)

Peters, W. K. and P. R. Bowlan. Single-shot Measurement of Extreme Ultraviolet Free Electron Laser Pulses And a few other measurements using ultrafast, short-wavelength lasers. . (LA-UR-20-25717)

Posters

Jones, T. N., W. K. Peters, R. L. Sandberg and P. R. Bowlan. Measuring Femtosecond Extreme-Ultraviolet Pulses With Slow Visible Cameras. Presented at *LANL Annual Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27709)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. Single-shot, all-optical complete electric field measurement of extreme ultraviolet free electron laser pulses. Presented at *2020 Virtual SSRL/ LCLS Users' Meeting*, Menlo Park, California, United States, 2020-09-28 - 2020-10-09. (LA-UR-20-27432)

Peters, W. K., T. N. Jones, P. R. Bowlan and R. L. Sandberg. Nonlinear Optics with Ionizing Radiation and Ultrafast Lasers: Progress Toward Measuring the Complete Electric Field of XFEL Pulses. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28443)

Tuning Functionality via Dimensionality in 4f-Based Nanowires

Priscila Rosa
20190076ER

Project Description

This project directly addresses a basic research need for energy and security relevant technology by providing the science required to discover, understand and ultimately control nanostructured forms of matter. Our approach is enabled by the ability to exploit low-dimensional correlated systems to tune functionality. Not only addressing a fundamental problem that is unexplored experimentally, this project also brings a new capability of probing 4f-based nanowires that will enable understanding and control of new materials and new physics that may emerge in the future.

Shockwave Metamaterials: Harnessing Structural Hierarchy for Tailorable Dynamic Response

Dana Dattelbaum
20190084ER

Project Description

Structural materials that function extensively as structural supports and protective components in aerospace and military applications are poised for transformational improvements through an ability to control structure with the advent of additive manufacturing. To date, these advances have been almost entirely related to tailorable mechanical response with only a limited number of studies interrogating the performance of these materials under the high strain rate-deformation, extreme conditions relevant to conventional and nuclear weapons environments. This project aims to lead the development of novel materials through dynamic characterization, materials modeling at high strain rates, along with the high resolution printing capabilities in order to understand the behavior of additively manufactured (AM) materials and their ability to tailor shockwave propagation offering a new class of materials for future stockpile applications.

Publications

Journal Articles

*Dattelbaum, D. M., A. Ionita, B. M. Patterson, B. A. Branch and L. Kuettner. Shockwave dissipation by interface-dominated porous structures. 2020. *AIP Advances*. **10** (7): 75016. (LA-UR-20-23537 DOI: 10.1063/5.0015179)

Dattelbaum, D. M., B. Branch, A. Ionita, B. M. Patterson and L. A. Kuettner. Shockwave interactions with additively-manufactured polymer structures. Submitted to *AIP Conference Proceedings*. (LA-UR-19-27099)

Presentation Slides

Dattelbaum, D. M., B. Branch, A. Ionita, B. M. Patterson and L. A. Kuettner. Shockwave interactions with additively-manufactured polymer structures (U). Presented at *2019 American Physical Society Shock Compression of Condensed Matter Topical Group meeting*, Portland, Oregon, United States, 2019-06-16 - 2019-06-22. (LA-UR-19-25436)

Air-Buoyant Vessel

Miles Beaux
20190119ER

Project Description

Remote sensing payloads, suspended from weather balloons for nonproliferation and treaty verification (as well as other surveillance applications), represent a potentially cheaper alternative to orbital satellite payloads. However, these ballooning applications face challenges such as the ever-increasing cost and decreasing supply of helium, the difficulty and cost of transporting helium, and the tendency of payloads to come down in undesirable locations which can be problematic for sensitive surveillance applications. This project aims to produce an air buoyant vacuum vessel (aka a vacuum balloon) as a helium-free alternative to weather balloons for suborbital atmospheric payload deployment. By utilizing a vacuum vessel filled with "nothing" instead of helium, it is expected that more permanent payload deployment can be achieved while greatly reducing the cost and providing better control over targeted location decent. This will be accomplished by developing ultra-light weight super-strong materials to meet the stringent engineering requirements for an air buoyant solid structure to be viable.

Publications

Presentation Slides

Hanson, C. J., S. L. Edwards and C. E. Hamilton. Additive Manufacturing and Novel Drying Methods Increase Accessibility and Decrease Integration Costs for Polyimide Aerogels. Presented at *5th Cross JOWOG on Additive Manufacturing*, Livermore, California, United States, 2020-01-27 - 2020-01-27. (LA-CP-20-20038)

Other

Ambrosiano, N. W. and M. F. I. Beaux. Balloon protype images. Audio/Visual. (LA-UR-20-27447)

Strongly Interacting Polariton Condensates at Room Temperature

Jinkyoung Yoo
20190224ER

Project Description

Quantum information science and technology will bring disruptive methods of information security, such as quantum computers powerful enough to break current encryption codes and quantum cryptography to prevent eavesdropping. However, the future is speculative because of the absence of suitable physical constituents for quantum information carriers. Current candidates for quantum information carriers do not fulfill the requirements of scalability, controllability, and robustness concurrently. Moreover, a few promising candidates require huge energy consumption due to quantum behaviors at cryogenic temperatures. This project aims at realizing robust and controllable quantum information carriers at room temperature in large scale. The physical constituents of the information carriers are interacting polariton condensates. Interacting polariton condensates will be made in semiconductor micro/nanocavity arrays embedding atomically thin quantum emitters. Interactions between polariton condensates can be controlled by external inputs. Thus, interacting polariton condensates can be used for computation. The system will be scalable due to the solid-state semiconductor platform -- a marked advantage over existing electronic systems. Additionally, polariton condensates are stable at room temperature. The expected deliverables will be breakthroughs in realization and deployment of quantum information systems.

Publications

Journal Articles

*Jeong, J., Q. Wang, J. Cha, D. K. Jin, D. H. Shing, S. Kwon, B. K. Kang, J. H. Jang, W. S. Yang, Y. S. Choi, J. Yoo, J. K. Kim, C. Lee, S. W. Lee, A. Zakhidov, S. Hong, M. J. Kim and Y. J. Hong. Remote heteroepitaxy of GaN microrod heterostructures for deformable light-emitting diodes and wafer recycle. 2020. *Science Advances*. **6** (23): eaaz5180. (LA-UR-19-29399 DOI: 10.1126/sciadv.aaz5180)

Kim, Y., T. Kim, J. Lee, Y. S. Choi, J. Moon, S. Y. Park, T. H. Lee, H. K. Park, S. A. Lee, M. S. Kwon, H. Byun, J. Lee, M. Lee, B. H. Hong and H. W. Jang. Tailored Graphene Micropatterns by Wafer-Scale Direct Transfer for Flexible Chemical Sensor Platform. 2020. *Advanced Materials*. 2004827. (LA-UR-20-29018 DOI: 10.1002/adma.202004827)

Presentation Slides

Kim, Y., S. Swarnadeep, T. Ahmed, J. Jeong, S. Choi, Y. J. Hong, H. W. Jang, W. S. Yang and J. Yoo. Van der Waals epitaxy of germanium on multi-layer graphene/h-BN stacks: Limitation of screening out-of-plane dipole moment. Presented at *2020 MRS Virtual Spring/Fall meeting*, Online, New Mexico, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-29017)

Yoo, J. Two-dimensional Materials Research at LANL. . (LA-UR-19-27080)

Yoo, J. Multi-dimensional van der Waals heterostructures. Presented at *31st Rio Grande Symposium on Advanced Materials*, Albuquerque, New Mexico, United States, 2019-09-16 - 2019-09-16. (LA-UR-19-29194)

Yoo, J. 2D/3D van der Waals heterostructures. Presented at *2019 Materials Research Society Fall Meeting*, Boston, Massachusetts, United States, 2019-12-02 - 2019-12-02. (LA-UR-19-31957)

Yoo, J. Nucleation control in van der Waals epitaxy. Presented at *2020 Materials Research Society Spring/Fall virtual meeting*, Boston, Massachusetts, United States, 2020-11-29 - 2020-11-29. (LA-UR-20-29297)

Posters

Yoo, J. Semiconductor Nano-heterostructures Research at CINT. . (LA-UR-19-24208)

Accelerated Aging of Crystalline Plutonium Compounds

Justin Cross
20190228ER

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 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 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.

Wavelength-Selectable, Electrically Driven Single-Photon Sources Operating at Room Temperature

Istvan Robel
20190236ER

Project Description

Despite its clear potential to revolutionize secure communications, the implementation of quantum cryptography is stymied by the lack of practical technologies for generating single-photons. To address this, we will develop wavelength-selectable, electrically driven, room-temperature single photon sources that exploit the unique atomic-like yet size-tunable character of electronic states in colloidal semiconductor nanocrystals. This project will leverage our recent advances in demonstrating structure-based control over recombination processes in nanomaterials in the context of electroluminescent devices. Specifically, we will develop single-nanocrystal light-emitting diodes, and use them to demonstrate a new type of room-temperature single-photon source with wavelength-selectable emission as dictated by a particular application. Successful combination of our nanomaterials and device advances, resulting in the first practical single-photon sources, will have a game-changing impact in the field of quantum information by making them as common as blue or white light-emitting diodes (LEDs), ushering in a new era of rigorous cybersecurity and ubiquitous quantum computation.

Thermally Expandable Microspheres for Plastic-bonded Explosive (PBX) Properties Control

Amanda Duque
20190342ER

Project Description

This project aims to develop a high explosive system with shock sensitivity that may be controlled "on-demand". We will incorporate a small fraction (<1 wt%) of thermally expandable microspheres (TEMs) during the manufacturing process of the plastic-bonded explosive (PBX). The remainder of the explosive fabrication process would follow normally (i.e. pressing, casting, machining, etc), and the resulting PBX material would be in the "lower state" of shock sensitivity. That is, it would be less sensitive to insult, in particular an incoming shock wave. After exposure to a thermal stimulus (at a minimum temperature, which may be tuned by the properties of the TEM that is incorporated), either from the environment or electromagnetic energy, the TEMs would expand and decrease the local density. This creates an increase in the size and number of voids in the material, which will ultimately result in an increase in shock sensitivity. Thus, the material remains in a safer configuration until after exposure to the thermal stimulus, resulting in true "on-demand" control of explosives sensitivity.

Publications

Journal Articles

Duque, A. L., B. M. Patterson, L. A. Kuettner, S. R. Robillard, J. T. Mang and W. L. Perry. Novel PBX Formulations Containing Thermally-Expandable Microspheres for On-Demand Control of Explosive Behavior. Submitted to *AIP Conference Proceedings*. (LA-UR-19-26869)

S. Mehana, M. Z. and M. Fahes. Molecular Simulation Study of Low salinity Waterflooding Mechanisms. Submitted to *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. (LA-UR-20-20808)

Presentation Slides

Duque, A. L., B. M. Patterson, L. A. Kuettner, S. R. Robillard, J. T. Mang and W. L. Perry. Novel PBX formulations containing thermally-expandable microspheres for on-demand control of explosive behavior. Presented at *21st Biennial APS Topical Group on Shock Compression*, Portland, Oregon, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25321)

Patterson, B. M., K. C. Henderson, N. L. Cordes, L. A. Kuettner, T. A. Shear, P. M. J. Welch, C. F. Welch, M. J. Herman, J. S. Carpenter, C. J. Montgomery, A. Ionita, N. Chawla, J. J. Williams, K. Fezzaa, T. Sun and X. Xiao. Probing Material Morphology and Deformation as a Response to In situ Loading using X-ray Tomography. Presented at *Microscopy and Microanalysis 2019*, Portland, Oregon, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27238)

Emergent Bogoliubov Fermi Surface in Unconventional Superconductors

Roman Movshovich
20190360ER

Project Description

This research will develop a new tool for superconductivity research, opening a new window into the structure of the superconducting order parameter. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion, iron-based, and high temperature cuprate superconductors.

Publications

Journal Articles

Fan, Z., G. Chern and S. Lin. Enhanced Superconductivity in Quasi-periodic Crystals. Submitted to *Physical Review Letters*. (LA-UR-20-23148)

Kumar, U. and S. Lin. Inducing and controlling superconductivity in Hubbard honeycomb model using an electromagnetic drive. Submitted to *Physical Review B*. (LA-UR-20-30127)

Lin, S., D. Y. Kim, E. D. Bauer, F. Ronning, J. D. Thompson and R. Movshovich. Interplay of the spin density wave and a possible Fulde-Ferrell-Larkin-Ovchinnikov state in CeCoIn5 in rotating magnetic field. Submitted to *Physical Review Letters*. (LA-UR-20-23614)

Organic Molecular Electrocatalysts for Hydrogen Evolution Reaction

Piotr Zelenay
20190420ER

Project Description

This project targets an entirely new class of organic molecular electrocatalysts (OMECs) for hydrogen evolution reaction (HER), an electrochemical process of fundamental importance to the future large-scale hydrogen production and processing, powered by renewable energy. The primary objectives of this work are to understand the underlying HER mechanism at metal-free OMECs, identify the structure-activity relationship for heterocyclic molecules, and enable rational design of future HER catalysts. The proposed research originates from the Laboratory's discovery of the world's first highly active OMEC for hydrogen evolution reaction that, in addition to high activity, exhibits excellent durability in an acidic polymer. In this project, the OMEC performance will be enhanced through a combination of experiments and computational modeling-guided catalyst discovery. This research is expected to conclude in a radical departure from HER electrocatalysis based on metals, either precious or non-precious. It will offer an alternative and cost-effective path to catalyzing hydrogen evolution reaction, which is essential for hydrogen production and purification. This research stands a unique chance of making a significant impact in the fields of electrocatalysis, chemistry, materials science and energy technology, in agreement with Department of Energy goals in energy conversion, including development of materials for clean-energy applications.

Publications

Journal Articles

*Yin, X., L. Lin, U. Martinez and P. Zelenay. 2,2#-Dipyridylamine as Heterogeneous Organic Molecular Electrocatalyst for Two-Electron Oxygen Reduction Reaction in Acid Media. 2019. *ACS Applied Energy Materials*. **2** (10): 7272-7278. (LA-UR-18-27879 DOI: 10.1021/acsaem.9b01227)

Presentation Slides

Yin, X. Advancing Electrocatalysts for Energy and Environmental Applications. . (LA-UR-20-20432)

Yin, X., H. Gao, E. F. Holby and P. Zelenay. Structure-Activity Data Mining for Hydrogen Evolution Reaction at Organic Molecular Electrocatalysts. Presented at *235th ECS Meeting*, Dallas, Texas, United States, 2019-05-26 - 2019-05-30. (LA-UR-19-24898)

Posters

Yin, X. Organic Molecular Electrocatalysts for Energy-Water Nexus. Presented at *2019 AIChE Annual Meeting*, Orlando, Florida, United States, 2019-11-10 - 2019-11-15. (LA-UR-19-32632)

Magnetization Fluctuation Spectroscopy as a Dynamic Probe of Emergent Magnetic Phases

Scott Crooker
20190430ER

Project Description

Magnetic materials form the basis for a huge number of essential technological applications -- for example, magnetic information storage (disk drives), certain information processing schemes (magnetic random-access memory), and sensors. New magnetic materials with exotic and potentially useful new properties are continually being developed round the world. Understanding the physics that underpins the behavior of new magnetic materials is essential if a new material is ever to be adopted as a new technology. Traditionally, this physics is revealed using conventional 'perturbative measurements', wherein the material is excited, driven, or otherwise perturbed away from equilibrium, and its response back to equilibrium is measured. Our project will establish a new and entirely alternative means of revealing the physics of magnetization dynamics -- not based on perturbation, but rather on detecting the intrinsic and ubiquitous fluctuations that naturally exist in every magnetic material. This "magnetization noise" necessarily encodes the same information (as guaranteed by the famous Fluctuation-Dissipation Theorem), and can be used to reveal the underlying magnetization dynamics without ever perturbing the system away from equilibrium, which can be particularly important near magnetic phase transitions.

Publications

Journal Articles

Bian, M., A. Kamenskii, S. A. Crooker and H. Zeng. Atomically-thin Cr2Te3 Ferromagnet - a 2D Half-Metal. Submitted to *Nano Letters*. (LA-UR-20-26568)

*Chernyak, V. Y., F. Li, C. Sun and N. A. Sinitsyn. Integrable multistate Landau–Zener models with parallel energy levels. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (29): 295201. (LA-UR-20-20621 DOI: 10.1088/1751-8121/ab9464)

Crooker, S. A., P. Schiffer, M. M. Goryca, C. Nisoli, J. Li, C. Leighton, X. Zhang, J. Watts and A. Balk. Field-Induced Monopole Plasma in Artifcial Spin Ice. Submitted to *Nature*. (LA-UR-20-24139)

Nisoli, C. The Colored Noise of Spin Ice: Subdiffusion of Magnetic Monopoles in a Coevolving Vacuum. Submitted to *Applied Physics Letters*. (LA-UR-20-24778)

Nisoli, C. Topological order of the Rys F-model and its breakdown in realistic square spin ice: Topological sectors of Faraday loops. 2020. *EPL (Europhysics Letters)*. **132** (4): 47005. (LA-UR-20-20959 DOI: 10.1209/0295-5075/132/47005)

Yan, B., V. Y. Chernyak, W. H. Zurek and N. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. Submitted to *Physical Review Letters*. (LA-UR-20-26742)

Yan, B. and N. Sinitsyn. Recovery of damaged information and the out-of-time-ordered correlators. Submitted to *Physical Review Letters*. (LA-UR-20-22064)

Presentation Slides

Crooker, S. A. Listening to spin and magnetization noise. . (LA-UR-20-29529)

Mixed Conductors for Enhanced Fuel Cell Performance

Yu Seung Kim
20190440ER

Project Description

This project addresses energy security issues by improving the performance and reducing the cost of zero-emission energy conversion devices. The goal of the research is to develop improved catalyst supports for fuel cell applications. By enabling the support to conduct electrons and protons at the same time, we will enable higher performance with lower cost, leading to accelerated deployment of fuel cell technology for transportation and defense applications.

Publications

Journal Articles

Li, D., Y. Pan, X. Wang, C. Wang, Y. S. Kim and J. S. Spendelow. Effect of the Catalyst Metal Content on PEMFC Durability. Submitted to *ECS Transactions*. (LA-UR-19-27318)

Three-dimension (3-D) Printed Hierarchically Porous Heat Pipe Wicks

Matthew Lee
20190463ER

Project Description

This project aims to develop a new class of heat transfer materials with enhanced properties and performance metrics suitable for a wide range of engineering applications. Using three-dimensional (3-D) printing techniques recently pioneered by members of our team, the goal of this project is to generate novel metallic wicking materials for heat pipes with optimized structural geometries and a vastly broadened design space.
Heat pipes are key components in many technologies pertinent to the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) and other government agencies, including waste heat recovery, nuclear energy, space applications and high performance computing. Therefore, this research directly addresses current national security challenges in energy security, aerospace and defense applications. In addition, this research can potentially lead to the large-scale manufacturing of more compact and efficient heat pipe designs with increased capacity to transport thermal energy, thereby broadening the span of their end-use applications and advancing key technologies already used through the DOE complex and beyond. Through our research we aim to identify key parameters governing heat pipe performance, optimize these through the use of 3-D printing, and pave the way toward new heat pipe designs and applications that were not possible until now.

Direct Plutonium-239 Nuclear Magnetic Resonance: A Unique Tool for Understanding Plutonium

Eric Bauer
20200045ER

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.

Superdetonation Shaped Charges

Shawn Mcgrane
20200124ER

Project Description

Shaped charges are widely used by the military to defeat armor, breach barriers, and destroy unexploded ordnance. Shaped charges are also widespread in oil and gas well perforation. Due to these prominent applications, there has been continuous research into new methods of improving shaped charge capabilities. We recently patented an idea to use the phenomenon of superdetonation to increase explosive performance for shaped charge applications. While the detonation velocity of nitromethane is 6.2 kilometers per second (km/s), the superdetonation velocities can be up to 13 km/s. This is substantially higher than currently available high performance explosives, that have detonation velocities up to ~9 km/s. We will build, test, and optimize the first explosively driven shaped charges that use superdetonation to nearly double the performance of currently available explosives.

Plutonium-239 Nuclear Magnetic Resonance Studies of Aging and Defects

Filip Ronning
20200125ER

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.

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)

Presentation Slides

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)

Dynamics of Quantum Phase Transitions

Wojciech Zurek
20200156ER

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.

Publications

Journal Articles

Suzuki, F., M. Leneshko, W. H. Zurek and R. V. Krems. Localization of composite quantum particles in a random potential. Submitted to *Physical Review B*. (LA-UR-20-28806)

Yan, B., V. Y. Chernyak, W. H. Zurek and N. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. Submitted to *Physical Review Letters*. (LA-UR-20-26742)

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., H. Zeng, C. ZIa and H. Zhang. Dynamics of spontaneous symmetry breaking in a holographic superconductor. Submitted to *Nature Physics*. (LA-UR-19-31918)

Zurek, W. H., J. Stefaniak, A. Sinha, A. Francuz and D. Sadhukhan. Sonic horizons and casusality in the phase transition dynamics. Submitted to *Physical Review B*. (LA-UR-19-30546)

Books/Chapters

Zurek, W. H. Conscious of a Classical World in a Quantum Universe. (LA-UR-20-28307)

Presentation Slides

Zurek, W. H. Dynamics of Quantum Phase Transitions. . (LA-UR-20-29719)

Plutonium Elasticity at Extreme Pressures using Gigahertz Ultrasound in a Diamond Anvil Cell

Blake Sturtevant
20200198ER

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.

Predicting the Impact Sensitivity of New Explosives through Statistical Modeling

Virginia Manner
20200234ER

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.

Publications

Journal Articles

Cawkwell, M. J. and V. W. Manner. Atom equivalent energies for the rapid estimation of the heat of formation of explosive molecules with density functional tight binding theory. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-20-21254)

I. 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. Submitted to *Industrial & Engineering Chemistry Research*. (LA-UR-20-30351)

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)

Shedding Light on Quantum Phenomena in Topological Chiral Crystals

Rohit Prasankumar
20200240ER

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.

Publications

Journal Articles

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)

Sirica, N. S., P. Orth, M. Scheurer, Y. Dai, M. C. Lee, P. Padmanabhan, L. M. T. Mix, L. X. Zhao, G. Chen, B. Xu, R. Yang, B. Shen, C. C. Lee, H. Lin, S. A. Trugman, J. Zhu, 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. Submitted to *Nature Materials*. (LA-UR-20-23580)

Sirica, N. S. and R. P. Prasankumar. Shaking up topology with light. Submitted to *Nature Materials*. (LA-UR-21-20965)

Presentation Slides

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)

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)

Transition Metal Nitrides for Efficient Nitrogen Electrocatalysis

Rangachary Mukundan
20200294ER

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.

Publications

Journal Articles

Mukundan, R., G. Pilania, k. ramaiyan, A. Banerjee, C. Kreller and B. M. Ceballos. Roads Less Traveled: Nitrogen Reduction Reaction (NRR) Catalyst Design Strategies for Improved Selectivity. 2021. *Current Opinion in Electrochemistry*. 100723. (LA-UR-20-25145 DOI: 10.1016/j.coelec.2021.100723)

Posters

Ramaiyan, K., S. Komini Babu, C. Kreller, R. Mukundan, Y. S. Kim, S. Maurya, F. H. Garzon, S. Ozden, A. Benavidez and D. Kelly. Electrochemical Synthesis of Ammonia Using Origami-like Molybdenum Carbide Nanoflakes As Nitrogen Reduction Reaction Catalyst. Presented at *GRC - Electrochemistry*, Ventura, California, United States, 2020-01-04 - 2020-01-10. (LA-UR-19-32701)

Design Principles for Skyrmions in f-electron Materials

Shizeng Lin
20200357ER

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 f-electron materials. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion materials and spintronics.

Publications

Journal Articles

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)

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)

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)

Presentation Slides

Lin, S., S. M. Thomas and P. Ferrari Silveira Rosa. LDRD appraisal: Design Principles for Skyrmions in f- electron Materials. . (LA-UR-20-29340)

Posters

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)

Pushing Past the 100 Tesla Threshold: Designing a High Conductivity/High Strength Metallic Composite Conductor

John Carpenter
20200375ER

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.

Emergent Infrared Localized Surface Plasmon Resonances in Doped Spinel Metal Oxide Nanomaterials

Jennifer Hollingsworth
20200407ER

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 3-Dimensional 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.

Publications

Journal Articles

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)

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., 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)

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)

Measurement of Dynamic Friction via Kolsky Bar

Benjamin Morrow
20200418ER

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.

Publications

Journal Articles

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. Limiting Retained Austenite Decomposition in Quenched and Tempered Steel: Influences of Rapid Tempering and Silicon. Submitted to *ISIJ International*. (LA-UR-20-23093)

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)

Defects and Functional Interfaces for Desalination

Jacob Spendelow
20200425ER

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).

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., Q. Kang, S. Komini Babu, J. B. Waugh and J. S. Spendelow. Numerical Modelling of Ion Transport and Adsorption in Porous Media: A Two-scale Study for Capacitive Deionization Desalination. Submitted to *International Journal of Heat and Mass Transfer*. (LA-UR-20-25564)

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)

Additive Manufacturing of 3-Dimensional and Graded Density Explosive Structures

Dana Dattelbaum
20200632ER

Project Description

The development of Additive Manufacturing technologies for the production of High Explosive (HE) charges has allowed for the introduction of new functionalities into previously brute force materials. The discovery of mechanisms to introduce directional sensitivity, detonation steering and control and structurally mediated initiation regions promise the development of safer and more useful explosive charges. With previous work having discovered methods of introducing such functionality, more exploration is necessary to fully exploit the extensive possibilities enabled by this new manufacturing technique.

Publications

Presentation Slides

Brown, C. B. Microstructure Characterization of Additive-Manufactured PBX. . (LA-UR-20-22869)

Synchrotron-based High-Energy Proton Radiography

Matthew Freeman
20200644ER

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.

Publications

Reports

Freeman, M. S. PRIOR: Proton Microscope for FAIR. Shock Wave Experiements with PRIOR.. Unpublished report. (LA-UR-20-25617)

Quantitative Understanding of Electronic Correlations in F-Electron Quantum Matter

Shizeng Lin
20180098ER

Project Description

Understanding and ultimately predicting the properties of complex materials is required to secure US energy independence and bolster national security. This project, in particular, addresses the DOE priority of realizing controlled functionality by employing quantum materials that exhibit tunable and emergent properties driven via collective behavior of electrons. This class of materials holds strong promise for future applications ranging from power management and transmission, to quantum computation, to novel versatile sensors as emphasized in the recent DOE/BES Basic Research Needs reports “Quantum Materials for Energy Relevant Technology”. Our approach combines advanced neutron scattering methods with new approaches in modeling to quantitatively understand the link between collective electron behavior and materials properties, thus laying the scientific foundation that will enable predictive quantum matter design. The use of neutron scattering at high pressure as we will employ here, and science enabling material by design capabilities is of particular interest to the DOE/Office of Basic Energy Sciences. Finally, we note that properties of plutonium metal, which are of relevance to the NNSA stockpile stewardship and nuclear weapons missions, are also determined by collective electronic behavior. The research performed here will provide insights relevant to the understanding of plutonium.

Technical Outcomes

This project found several interesting physical phenomena enabled by strong electronic correlation in prototypical f-electron materials. This includes a stable Higgs boson in anisotropic quantum magnets, a large and tunable anomalous Hall conductivity, and strong evidence for the existence of Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. The results highlight the important role of strong electronic correlation as an organizing principle for novel quantum states.

Publications

Journal Articles

*Asaba, T., Y. Su, M. Janoschek, J. D. Thompson, S. M. Thomas, E. D. Bauer, S. Lin and F. Ronning. Large tunable anomalous Hall effect in the kagome antiferromagnet U3Ru4Al12. 2020. *Nature Communications*. **102** (3): 35127. (LA-UR-19-25889 DOI: 10.1103/PhysRevB.102.035127)

Fan, Z., G. Chern and S. Lin. Enhanced Superconductivity in Quasi-periodic Crystals. Submitted to *Physical Review Letters*. (LA-UR-20-23148)

*Halsbeck, F., S. Saeubert, M. Seifert, C. Franz, M. Schulz, A. Heinemann, T. Keller, P. Das, J. D. Thompson, E. D. Bauer, C. Pfleiderer and M. Janoschek. Ultrahigh-resolution neutron spectroscopy of low-energy spin dynamics in UGe2. 2019. *Physical Review B*. **99** (1): 014429. (LA-UR-18-20542 DOI: 10.1103/PhysRevB.99.014429)

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)

*Kim, T., C. Chien and S. Lin. Reentrant Fulde-Ferrell-Larkin-Ovchinnikov state in small-sized superconductors. 2019. *Physical Review B*. **99** (5): 054509. (LA-UR-18-30667 DOI: 10.1103/PhysRevB.99.054509)

Kumar, U., G. Price, K. Stiwinter, A. Nocera, S. Johnson and T. Datta. Spectroscopic signatures of the next-nearest-neighbor hopping in the charge and spin dynamics of doped one-dimensional antiferromagnets. Submitted to *Physics Review, ARXIV*. (LA-UR-20-22832)

*Li, S., Y. Su, Y. Ren and L. He. Valley Polarization and Inversion in Strained Graphene via Pseudo-Landau Levels, Valley Splitting of Real Landau Levels, and Confined States. 2020. *Science*. **124** (10): 106802. (LA-UR-19-21456 DOI: 10.1103/PhysRevLett.124.106802)

Lin, S., D. Y. Kim, E. D. Bauer, F. Ronning, J. D. Thompson and R. Movshovich. Interplay of the spin density wave and a possible Fulde-Ferrell-Larkin-Ovchinnikov state in CeCoIn5 in rotating magnetic field. Submitted to *Physical Review Letters*. (LA-UR-20-23614)

*Lin, S., J. Zhu and A. Saxena. Kelvin modes of a skyrmion line in chiral magnets and the associated magnon transport. 2019. *Physical Review B*. **99** (14): 140408. (LA-UR-19-20239 DOI: 10.1103/PhysRevB.99.140408)

Su, Y., A. Masaki-Kato, W. Zhu, J. Zhu, Y. Kamiya and S. Lin. Stable Higgs mode in anisotropic quantum magnets. Submitted to *Physical Review X*. (LA-UR-20-24832)

*Su, Y. and S. Lin. Nontrivial topology and localization in the double exchange model with possible applications to perovskite manganites. 2018. *Physical Review B*. **98** (23): 235116. (LA-UR-18-29965 DOI: 10.1103/PhysRevB.98.235116)

*Su, Y. and S. Lin. Pairing symmetry and spontaneous vortex-antivortex lattice in superconducting twisted-bilayer graphene: Bogoliubov-de Gennes approach. 2018. *Physical Review B*. **98** (19): 195101. (LA-UR-18-26090 DOI: 10.1103/PhysRevB.98.195101)

Su, Y. and S. Lin. Topological Sliding Moire \xcc\x81 Heterostructure. Submitted to *Physical Review Letters*. (LA-UR-19-30658)

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Presentation Slides

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *Annual Conference on Magnetism and Magnetic Materials*, Las Vegas, Nevada, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31136)

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21986)

Su, Y. Twisted bilayer graphene: topological pumping and switching of topology by current. . (LA-UR-20-24896)

Posters

Huang, Z., C. Ting, J. Zhu and S. Lin. Stable Higgs Modes in Fulde-Ferrell-Larkin- Ovchinnikov (FFLO) states. Presented at *CINT annual meeting*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-26. (LA-UR-19-29466)

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Making the Unmakeable: Nanostabilized Magnetic Alloys

Sergei Ivanov
20180114ER

Project Description

In recent years, there has been an explosion in recognizing the need for new low-cost rare-earth-free magnetic materials for various applications: hard ferromagnets, as ideal active components for a broad range of energy generating/converting devices, multiferroic (e.g., ferromagnetic and magnetoelectric) and ferromagnet/antiferromagnet composites for advanced electronic and spintronic circuitry components. Combination of light magnetic metals with electron-rich heavy elements, such as thallium (Tl), lead (Pb), or bismuth (Bi), has long been considered a lucrative goal in the search for such magnetic materials. The unfortunate problem of complete immiscibility of these metals at ambient pressures precluded the synthesis of such alloys. We propose a general path to overcome the miscibility limitation that will lead to the formation of those “forbidden” alloys of manganese (Mn), iron (Fe), or cobalt (Co) with Pb or Bi and their oxides via nanoscale synthesis. Once successfull, the project will demonstrate the low-cost, general, and facile approach to hard-to-synthesize metal alloys for multiple applications. In particular, it will open up a path toward unique magnetic materials necessary for efficient energy generation and new generation of circuitry components for electron spin manipulation. The latter would lead to novel secure computing approaches, sensors, and other magnetoelectronics-based devices.

Technical Outcomes

This project clearly established the factors limiting the formation of 3-dimensional (3d) metals with lead (Pb) and bismuth (Bi). In the process, the team developed the use of a single type ligand (protecting molecule) to generate the source of 3d metal in the reaction. Using this technique, the team developed a unified approach to the synthesis of a library of MSn(x) and MSb(x) (M=Cr-Ni) alloys. This project also established the limitations to a commonly used method of alloy synthesis and presented the explanation for these limitations.

Publications

Posters

Li, M. M. and S. A. Ivanov. Layered Ternary Chalcogenide Nanoparticles towards Supercapacitor Applications. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28807)

McGrath, A. J. and S. A. Ivanov. Magnetic M-Sb and M-Sn2 (M = Mn, Fe, Co) intermetallic nanocrystals from metal amidinate precursors. Presented at *LANL Postdoc Symposium*, Los Alamos, New Mexico, United States, 2018-08-27 - 2018-08-27. (LA-UR-18-27978)

McGrath, A. J. and S. A. Ivanov. Metal amidinates as precursors for transition metal-based intermetallic nanocrystals. Presented at *LANL 2019 Postdoc Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28516)

Next Generation Discrete Dislocation Dynamics Modelling for Materials Science Applications

Laurent Capolungo
20180250ER

Project Description

Having the ability to model microstructure-sensitive behavior of materials is essential to predict performance and to design new materials. The proposed work will improve the physics underlying polycrystalline materials models and, at the same time, provide a robust method to quantify defect content with non destructive evaluation (NDE). NDE methods are typically used to probe the state of material systems in service conditions. These approaches are particularly pertinent in scenarios in which the material is subjected to harsh environments (pressure, radioactivity, etc.). The project will largely contribute to vetting NDE based assessment of the material state and performance in harsh conditions.

Technical Outcomes

Developments pertaining to resonance ultrasound spectroscopy (RUS) and to diffraction line profile analysis (LPA) both significantly advanced the field of non-destructive materials characterization. This project demonstrated that new microstructural information can be extracted from RUS, and delivered a tool to make LPA easier to use for the diffraction community.

Publications

Journal Articles

Bamney, D., A. E. Tallman, L. Capolungo and D. E. Spearot. Virtual diffraction analysis of dislocations and dislocation networks in discrete dislocation dynamics simulations. Submitted to *Computational Materials Science*. (LA-UR-20-27556)

*Berbenni, S., V. Taupin and R. A. Lebensohn. A fast Fourier transform-based mesoscale field dislocation mechanics study of grain size effects and reversible plasticity in polycrystals. 2020. *Journal of the Mechanics and Physics of Solids*. **135**: 103808. (LA-UR-19-31410 DOI: 10.1016/j.jmps.2019.103808)

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Evans, J. E., B. Sturtevant, B. Clausen, S. C. Vogel, F. F. Balakirev, L. Capolungo, R. A. Lebensohn and B. A. Maiorov. Determining Elastic Anisotropy of Textured Polycrystals using Resonant Ultrasound Spectroscopy. Submitted to *Journal of Materials Science*. (LA-UR-20-26566)

*Gen\xc3\xa9e, J., S. Berbenni, N. Gey, R. A. Lebensohn and F. Bonnet. Particle interspacing effects on the mechanical behavior of a Fe–TiB2 metal matrix composite using FFT-based mesoscopic field dislocation mechanics. 2020. *Advanced Modeling and Simulation in Engineering Sciences*. **7** (1): 6. (LA-UR-19-31404 DOI: 10.1186/s40323-020-0141-z)

Kohnert, A. A. and L. Capolungo. Spectral Discrete Dislocation Dynamics with Anisotropic Short Range Interactions. Submitted to *Computational Materials Science*. (LA-UR-20-25289)

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2020. *International Journal of Plasticity*. **125**: 210-234. (LA-UR-19-31405 DOI: 10.1016/j.ijplas.2019.09.011)

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Wallis, D., L. Hansen, A. Wlikinson and R. A. Lebensohn. Dislocation interactions in olivine control postseismic creep of the upper mantle. Submitted to *Nature Communications*. (LA-UR-20-24462)

Reports

Lebensohn, R. A. Machine-learning-based reduced-order models for the relationship between aging and strength of self-irradiated materials.. Unpublished report. (LA-UR-20-23144)

Presentation Slides

Capolungo, L., A. E. Tallman, R. A. Lebensohn, A. A. Kohnert and A. K. Mariyappan. Combining micromechanical models and machine learning to build reduced-order models for advanced characterization and engineering applications.. Presented at *Discussion with NASA*, Los Alamos, New Mexico, United States, 2020-08-03 - 2020-08-03. (LA-UR-20-25328)

Evans, J. A. Nuclear Reactor Materials and Anisotropy. . (LA-UR-19-32212)

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Tallman, A. E., R. Pokharel and L. Capolungo. Discrete dislocation dynamics-based prediction of dislocation density from diffraction line profiles of Ta. Presented at *TMS Annual Meeting*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21678)

Posters

Christodoulou, P., A. F. Samuel, T. Francis, M. Echeverria, A. Needleman, T. Pollock, R. A. Lebensohn, F. Zok and I. Beyerlein. Mesoscale modeling of two-phase material deformation. Presented at *2019 Stewardship Science Academic Programs (SSAP) Annual Review Symposium*, Albuquerque, New Mexico, United States, 2019-02-19 - 2019-02-19. (LA-UR-19-21415)

Dopant Profiling in Semiconductors by Scanning Frequency Comb Microscopy

Dmitry Yarotski
20180283ER

Project Description

Moore's Law is a techno-economic model describing the tendency of nearly doubling the performance and functionality of digital electronics every two years within a fixed cost and area. Within a decade, it predicts that novel lithographic processes will bring characteristic device dimensions into the 3 nanometer (nm)–5 nm realm. This range corresponds to a dozen or fewer dopant atoms across critical circuit features, thus leading to the strong dependence of the device performance on the location of each impurity. Therefore, the progress in fabrication demands adequate characterization tools as it is no longer possible with current instrumentation for the semiconductor industry to satisfy the rule-of-thumb that the resolution in charge carrier profiling should be finer than 10% of the lithographic feature dimension, i.e. better than 1 nm. We will leverage recent Los Alamos National Laboratory breakthroughs in the development of nanoscale microwave sources, as well as extensive Laboratory capabilities in scanning probe microscopy and ultrafast laser spectroscopy to achieve non-destructive low-noise carrier profiling with unprecedented (~0.1 nm) resolution using newly-developed Scanning Frequency Comb Microscopy (SFCM). The primary benefit of our project would be improved semiconductor metrology that will facilitate further advances in semiconductor fabrication technologies and consumer electronics and computing.

Technical Outcomes

This project developed the first Scanning Frequency Comb Microscope to produce and detect broadband (>10 terahertz, THz) Microwave Frequency Combs from various surfaces at nanoscale resolution and attoWatt sensitivity. Although these characteristics do not yet meet the requirements for atomically resolved dopant profiling in semiconductors, the instrument will have scientific applications as a scanned sub-nanometer microwave source which sets the present state-of-the-art as a narrow linewidth microwave source having low-noise and high stability.

Publications

Journal Articles

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Presentation Slides

T. Mix, L. M., D. Ghosh, J. T. Tisdale, M. C. Lee, K. R. O'Neal, N. S. Sirica, A. J. Neukirch, W. Nie, R. P. Prasankumar and D. A. Yarotski. Recombination Dynamics of Chlorine Doped Hybrid Perovskite Single Crystals. Presented at *Virtual Cleo*, San Jose, California, United States, 2020-05-11 - 2020-05-15. (LA-UR-20-23422)

T. Mix, L. M., M. C. Lee, K. R. O'Neal, N. S. Sirica, D. Ghosh, J. T. Tisdale, W. Nie, R. P. Prasankumar and D. A. Yarotski. Recombination Dynamics of Chlorine Doped Hybrid Perovskite Single Crystals. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21964)

Yarotski, D. A. Probing and manipulating quantum materials with THz pulses. Presented at *LIGHT ON THE QUANTUM LEAP: XFELS FOR QUANTUM MATERIALS*, tempe, Arizona, United States, 2019-01-16 - 2019-01-19. (LA-UR-19-20432)

Posters

O'Neal, K. R., B. Kuthanazhi, N. H. Jo, S. L. Bud'Ko, P. C. Canfield, J. Zhu, P. Orth, A. J. Taylor, R. P. Prasankumar and D. A. Yarotski. Ultrafast Carrier Dynamics of EuCd2As2. Presented at *CATS EFRC Midterm Review*, Gaithersburg,

Maryland, United States, 2020-02-04 - 2020-02-04. (LA-UR-20-20524)

Two-dimensional Nanostructure-Engineered Durable Supercapacitors

Sergei Ivanov
20180360ER

Project Description

Supercapacitors are emerging energy storage devices complementary to conventional batteries, due to their shorter charging times, long lifetime, and wider temperature operational ranges. In addition, recent incidents have highlighted safety concerns surrounding the use of high energy density batteries due to the presence of highly reactive components. Supercapacitors are uniquely poised for applications such as regenerative breaking in cars, static random access memory, motor starters, and various electronics. However, current materials used in supercapacitors have inherent technical limitations. We propose structural modifications to ubiquitous layered molybdenum disulfide (MoS2) that will lead to the increase in performance of supercapacitors and to the improvement of the material's durability to prolonged use and handling. Specifically, our project will result in: (1) synthesis of nanocrystalline mix-metal layered copper sulfides or selenides with group VI metals or antimony (Sb) with molecular spacers between layers, (2) complete structural/electrochemical characterization of synthesized materials to establish the influence of composition, size and interlayer distance on their properties, and (3) fabrication of a durable supercapacitor prototype. Project success will lead to a new area of supercapacitor development using high performance low-cost materials coupled with ease of device manufacturing.

Technical Outcomes

The project succeeded in synthesizing mix-metal chalcogenides using a novel route. The introduction of spacers encountered a challenge of their alignment perpendicularly to structural layers. Instead, a new type of spacers, namely dithiol-ferrocene, has been synthesized. The electrochemical characterization of as-synthesized materials has revealed moderate electrochemical properties (with capacitance (C) of ~10 farads per gram), but exfoliation and introduction of ferrocene linker increased capacitance by five-fold each.

Publications

Journal Articles

Ivanov, S. A. and M. M. (. Li. 2D Nanocrystalline Ternary Selenides Cu2MSe4 (M=Mo/W). Submitted to *Dalton Transactions*. (LA-UR-20-27015)

*Li, M. M. and S. A. Ivanov. 2D nanocrystalline ternary selenides Cu MSe (M = Mo/W). 2019. *Dalton Transactions*. **48** (42): 15795-15801. (LA-UR-19-29655 DOI: 10.1039/C9DT03282G)

Presentation Slides

Li, M. M. and S. A. Ivanov. Syntheses of phase pure ternary layered chalcogenides of Mo and W. Presented at *ACS Fall 2019 National Meeting & Exposition*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-28100)

Li, M. M. and S. A. Ivanov. Syntheses of copper tetrachalcogenide metallate (Mo/W) nanoparticles: Applications towards energy storage. Presented at *ACS Southeastern Regional Meeting*, Savannah, Georgia, United States, 2019-10-19 - 2019-10-23. (LA-UR-19-30075)

Posters

Li, M. M. and S. A. Ivanov. Layered Ternary Chalcogenide Nanoparticles towards Supercapacitor Applications. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28807)

Li, M. M. and S. A. Ivanov. Solutional Nanoparticle Syntheses of Layered Ternary Copper Selenides of Mo/W. Presented at *Materials Research Society 2019 Fall Meeting*, Boston, Massachusetts, United States, 2019-11-30 - 2019-12-05. (LA-UR-19-31366)

Switchable Spin Crossover Explosives: Nitrogen-rich Iron (Fe II) Complexes for On-Demand Initiation Sensitivity

Jacqueline Veauthier
20180369ER

Project Description

We seek to develop explosive materials that can switch from a insensitive (safe) phase to a more sensitive (less safe) phase when exposed to the appropriate stimuli. In the insensitive state, these materials would greatly reduce the potential for accidental detonation, while in the sensitive state they could be reliably detonated. This proposal addresses a long-standing goal within the Department of Energy (DOE) and the Department of Defense (DOD) communities for explosive materials with on-demand sensitivity and successful development of these materials would put Los Alamos National Laboratory at the forefront of the insensitive munitions efforts. Technologies derived from the proposed research will contribute to National R&D needs for the prediction and control of explosive initiation and Laboratory core missions in stockpile stewardship and energetic materials science. Our materials by design approach will not only advance the fundamental science of explosives, but will also have a broad impact in designing other molecularly switchable photonic materials. Our work will produce high impact results, train the next generation of energetic materials scientists and theorists and will put the Laboratory at the forefront of explosives science.

Technical Outcomes

This project explored the spin crossover and explosive sensitivity properties of a new class of explosive spin crossover compounds (ExSCO) using both experimental and theoretical methods. These ExSCOs are based on a class of molecular complexes of iron with nitrogen-rich triazole ligands. The team demonstrated, for the first time, that there is a correlation between spin state and explosive impact sensitivity for the compound "[Fe(Htrz)3]n[ClO4]2n," which exhibits switchable impact sensitivity with a fully reversible switching mechanism.

Publications

Journal Articles

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Lanthanide Complexes of Bis(tetrazolato)amine: A Route to Lanthanide Nitride Foams. 2020. *Inorganic Chemistry*. **59** (22): 16109-16116. (LA-UR-19-28081 DOI: 10.1021/acs.inorgchem.0c02480)

Nguyen, T. D., J. M. Veauthier, D. E. Chavez, B. C. Tappan, A. H. Mueller, B. L. Scott and D. A. Parrish. Lanthanide Complexes of Bi(tetrazolato)amine: a New Route to Lanthanide Nitride Foams. Submitted to *Inorganic Chemistry*. (LA-UR-20-26062)

*Nguyen, T. D., J. M. Veauthier, G. F. Angles-Tamayo, D. E. Chavez, E. Lapsheva, T. W. Myers, T. R. Nelson and E. J. Schelter. Correlating Mechanical Sensitivity with Spin Transition in the Explosive Spin Crossover Complex [Fe(Htrz)3]n[ClO4]2n. 2020. *Journal of the American Chemical Society*. **142** (10): 4842-4851. (LA-UR-19-30677 DOI: 10.1021/jacs.9b13835)

Reports

Nelson, T. R., J. M. Veauthier, G. F. Angles-Tamayo and Y. Zhang. IC Annual Report. Unpublished report. (LA-UR-19-22530)

Presentation Slides

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Investigation of Explosive Spin Crossover Complexes for On-Demand Initiation Sensitivity and Energetic Polymers for Additive Manufacturing. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK19)*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25378)

Veauthier, J. M. Designing Energetic Coordination Complexes to Tune Explosive Initiation and Discover New Routes to Important Materials. Presented at *Inorganic Chemistry Gordon Research Conference*, Biddeford, Maine, United States, 2018-06-19 - 2018-06-19. (LA-UR-18-25262)

Veauthier, J. M. Nitrogen-rich metal coordination complexes for new applications in explosive initiation. Presented at *ACS Fall 2019 National Meeting*, San Diego, California, United States, 2019-08-25 - 2019-08-25. (LA-UR-19-28434)

Posters

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Development of Switchable Explosive Materials for the Additive Manufacturing of Insensitive Munitions. Presented at *Energetic Materials Gordon Research Conference*, Newry, Maine, United States, 2018-06-03 - 2018-06-03. (LA-UR-18-24723)

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Investigation of an Explosive Spin Crossover Complex for On-Demand Initiation Sensitivity and Energetic Polymers for Additive Manufacturing. Presented at *Agnew National Security and Metropolis Postdoc Fellow Showcase*, Los Alamos, New Mexico, United States, 2019-12-10 - 2019-12-10. (LA-UR-19-32236)

Breaking the Efficiency Limits in Quantum Dot Emitters Using Dual-Band Metamaterials

Houtong Chen
20180372ER

Project Description

Development of energy efficient materials and device architecture is one of the central missions of the Laboratory and our nation. Rational design of mesoscale and nanoscale materials and creation of transformative device concepts are critical to address some grand challenge questions regarding key technological gaps in photonics and optoelectronics (2012 National Research Council report). The success of this work will impact many quantum dot and thin-film optoelectronic applications, including thin film solar cells, high efficiency light emitting diodes (LEDs), ultrafast and sensitive detectors, to name a few. This project also leverages the fabrication, integration, and characterization capabilities at the Center for Integrated Nanotechnologies (CINT), a DOE national user facility.

Technical Outcomes

This project demonstrated a transformational concept of hybrid metamaterials by integrating colloidal quantum dots. The photoluminescence spectra exhibited ~50-fold enhancement when the metamaterial resonances coincided the quantum dot emission wavelengths. The angle-resolved radiation patterns of quantum dot photoluminescence matched the metamaterial absorption spectra, confirming the essential role of metamaterial resonances in photoluminescence enhancement. The team's additional experiments indicated strong metamaterial mediated spontaneous emission rate of quantum dots which is responsible for the photoluminescence enhancement.

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., J. Huang, X. Wang, D. Li, T. Jin, P. Lu, P. Lin, J. Narayan, X. Zhang and H. Wang. 3D Hybrid Plasmonic Framework with Au Nanopillars Embedded in Nitride Multilayers Integrated on Si. 2020. *Advanced Materials Interfaces*. **7** (17): 2000493. (LA-UR-20-28042 DOI: 10.1002/admi.202000493)

Chen, H., S. Misra, D. Zhang, Z. Qi, D. Li, J. Lu and H. Wang. Morphology control of self-assembled three-phase Au-BaTiO3-ZnO hybrid metamaterial for tunable optical properties. Submitted to *Crystal Growth & Design*. (LA-UR-20-28045)

*Huang, J., H. Wang, D. Li, Z. Qi, D. Zhang, P. Lu, H. Chen, D. A. Yarotski, P. Lin, X. Zhang and H. Wang. Room-Temperature Ferroelectric LiNb6Ba5Ti4O30 Spinel Phase in a Nanocomposite Thin Film Form for Nonlinear Photonics. 2020. *ACS Applied Materials & Interfaces*. **12** (20): 23076-23083. (LA-UR-20-28041 DOI: 10.1021/acsami.0c03487)

*Wang, C., T. G. Habteyes, T. S. Luk, J. F. Klem, I. Brener, H. Chen and O. Mitrofanov. Observation of Intersubband Polaritons in a Single Nanoantenna Using Nano-FTIR Spectroscopy. 2019. *Nano Letters*. **19** (7): 4620-4626. (LA-UR-19-22652 DOI: 10.1021/acs.nanolett.9b01623)

Presentation Slides

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversion. Presented at *The 9th International Symposium on Ultrafast Phenomena and Terahertz Waves (ISUPTW 2018)*, Changsha, China, 2018-04-23 - 2018-04-23. (LA-UR-18-23594)

Chen, H. Broadband Terahertz Linear-to-Circular Polarization Conversion. Presented at *IRMMW-THz 2018*, Nagoya, Japan, 2018-09-10 - 2018-09-10. (LA-UR-18-28683)

Chen, H. Active Metamaterials & Metasurfaces. . (LA-UR-19-24205)

Chen, H. Metasurfaces for Optical Antireflection and Bandpass Filters. Presented at *META 2019*, Lisbon, Portugal, 2019-07-23 - 2019-07-23. (LA-UR-19-27279)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversions. Presented at *MTSA 2019*, Busan, Korea, South, 2019-09-30 - 2019-09-30. (LA-UR-19-29968)

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)

Li, D., C. Chang, Z. Zhao, A. J. Taylor, S. Fan and H. Chen. Broadband Linear-to-Circular Polarization Converter based on Reflective Birefringent Metasurfaces. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21921)

Li, D., C. Chang, Z. Zhao, A. J. Taylor, S. Fan and H. Chen. Broadband Linear-to-Circular Polarization Converter based on Reflective Birefringent Metasurfaces. Presented at *CLEO*, San Jose, California, United States, 2020-05-11 - 2020-05-16. (LA-UR-20-23244)

Wang, C. The localized surface plasmonic effects: from far-field to near-field optical measurements. . (LA-UR-19-22548)

Posters

Li, D., C. Chang, A. Singh, J. A. Hollingsworth and H. Chen. Enhancing the Light Emission of Colloidal Quantum Dots with Perfect Absorbers Based on Metasurfaces. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21922)

Wang, C., H. Chen and O. Mitrofanov. Nano-FTIR Spectroscopy of Intersubband Transition in Single Plasmonic Nanoantenna Regime. Presented at *2019 LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-08. (LA-UR-19-27747)

Novel Algorithms for Large-Scale Ab-Initio Materials Simulations: Extending the Reach of Quantum Mechanics

Ondrej Certik
20180428ER

Project Description

The project significantly advances the capabilities of large-scale quantum mechanical materials calculations by developing, implementing, and applying a new class of real-space methods for solving the Kohn-Sham (KS) equations of Density Functional Theory (DFT). They will have broad applicability in condensed matter physics and molecular quantum mechanics by enabling ab initio quantum mechanical simulations of a wide range of large scale materials systems. They will also have the potential to be more efficient than the algorithms implemented in standard production codes like the Vienna Ab Initio Simulation Package (VASP) and "ABINIT," which are used for large-scale quantum-mechanical simulations using pseudopotentials. This would extend the applicability of Kohn-Sham pseudopotential DFT calculations to longer length and time scales in molecular dynamics, hence permitting new fundamental understanding and reliable prediction of macroscopic physical properties from ambient to extreme conditions. As such it advances mission challenges for agencies such as the National Nuclear Security Administration and has mission relevance to the Stockpile Stewardship Program, Explosives, lithium-ion batteries simulations (Commerce and Transportation and Renewable Energy) and others.

Technical Outcomes

This project implemented and validated a 3-dimensional flat-top partition-of-unity-method (FT-PUM) solver for Kohn-Sham equations and verified that this method requires an order of magnitude fewer degrees of freedom compared to the state-of-the-art plane wave methods in production codes. This fact dramatically speeds up the performance of the eigensolver which is the most expensive part of the electronic structure calculations using the density functional theory. This project's FT-PUM method paves the way for faster electronic structure calculations.

Publications

Journal Articles

Benvenuti, E., A. Chiozzi, G. Manzini and N. Sukumar. Extended virtual element method for the Laplace equation with singularities and discontinuities. Submitted to *Computer Methods in Applied Mechanics and Engineering*. (LA-UR-19-20877)

Manzini, G., F. Gardini and G. Vacca. The nonconforming virtual element method for eigenvalue problems. Submitted to *ESAIM: Mathematical Modelling and Numerical Analysis*. (LA-UR-20-27582)

Manzini, G., G. Maguolo and M. Putti. The high order mixed mimetic finite element method for time dependent diffusion problem. Submitted to *SIAM Journal on Numerical Analysis*. (LA-UR-17-28535)

Manzini, G., O. Certik, F. Gardini, L. Mascotto and G. Vacca. p- and hp-versions of the virtual element method for eigenvalue elliptic problems. Submitted to *Computers & Mathematics with Applications*. (LA-UR-20-27584)

Manzini, G., O. Certik, F. Gardini and G. Vacca. The virtual element method for eigenvalue problems with potential terms on polytopal meshes. Submitted to *Applications of Mathematics*. (LA-UR-18-21436)

Manzini, G., P. Antonietti and M. Verani. The conforming virtual element method for polyharmonic problems. Submitted to *Computers & Mathematics with Applications*. (LA-UR-20-27583)

*Beir\xc3\xa3o da Veiga, L., G. Manzini and L. Mascotto. A posteriori error estimation and adaptivity in hp virtual elements. 2019. *Numerische Mathematik*. **143** (1): 139-175. (LA-UR-18-23445 DOI: 10.1007/s00211-019-01054-6)

Reports

Certik, O., F. Gardini, G. Manzini, L. Mascotto and G. Vacca. Design, analysis and numerical experiments for the virtual element p and hp approximations of elliptic eigenvalue problems. Unpublished report. (LA-UR-18-31762)

Certik, O. and J. E. Pask. Why to Use Fortran For New Projects. Unpublished report. (LA-UR-19-24165)

Gardini, F., G. Manzini and G. Vacca. The nonconforming virtual element method for eigenvalue problems. Unpublished report. (LA-UR-18-20850)

Gyrya, V., G. Manzini, S. Naranjo-Alvarez and V. A. Bokil. The virtual element method for resistive magnetohydrodynamics: Design, wellposedness, stability, and preliminary numerical results.. Unpublished report. (LA-UR-19-31726)

Manzini, G., E. Benvenuti, A. Chiozzi and N. Sukumar. Numerical experiments with the extended virtual element method for the Laplace problem with strong discontinuities. Unpublished report. (LA-UR-18-23443)

Manzini, G., H. M. Mourad, P. F. Antonietti, I. Mazzieri and M. Verani. The arbitrary-order virtual element method for linear elastodynamics models. Convergence, stability and dispersion-dissipation analysis.. Unpublished report. (LA-UR-20-23773)

Manzini, G., H. M. Mourad, P. F. Antonietti and M. Verani. The virtual element method for linear elastodynamics models. Design, analysis, and implementation. Unpublished report. (LA-UR-19-29577)

Manzini, G., O. Certik, J. Droniou and N. Sukumar. The gradient discretization framework for virtual element and partition of unity methods for the Schrodinger equation. Unpublished report. (LA-UR-18-29148)

Manzini, G., P. F. Antonietti and M. Verani. Design and convergence analysis of the conforming virtual element method for polyharmonic problems. Unpublished report. (LA-UR-18-29151)

Manzini, G. and G. Vacca. Design, analysis and preliminary numerical results for the nonconforming VEM for parabolic problems. Unpublished report. (LA-UR-18-29150)

Presentation Slides

Certik, O., G. Manzini, L. A. Collins, N. Sukumar, J. E. Pask and M. A. Schweitzer. Flat-top Partition of Unity Method for Electronic Structure Calculations. Presented at *WCCM 2018*, New York City, New York, United States, 2018-07-23 - 2018-07-27. (LA-UR-18-26760)

Certik, O., G. Manzini, L. A. Collins, N. Sukumar, J. E. Pask and M. A. Schweitzer. Flat-top Partition of Unity Method for Electronic Structure Calculations. Presented at *WCCM 2018*, New York City, New York, United States, 2018-07-23 - 2018-07-27. (LA-UR-18-26905)

Methods and Algorithms to Account for Field Fluctuations Obtained by Homogenization in Solid Mechanics

Ricardo Lebensohn
20180441ER

Project Description

Los Alamos National Laboratory is a world leader in the theoretical formulation and numerical implementation of physically-based materials models of plasticity and failure of crystalline materials. We have pioneered the coupling of these models with numerical solutions based on Finite Elements (FE), resulting in numerical models at the engineering scale with sensitivity to the material's microstructure. These capabilities are part of the long-term objective of the Laboratory, critical to its stewardship mission. This project will explore one possible avenue to realize the theoretical and numerical counterparts of critical experiments related to the science of matter in extremes, crystalline material deformation with the goal of parameterizing and validating multiscale models. We will advance existing numerical tools, enabling mid-term practical applications to present problems faced by different experimental and modeling groups within the Laboratory.

Technical Outcomes

This project successfully developed the theory, methods, and algorithms to systematically account for the effect of field fluctuations on microstructure evolution of polycrystalline materials within the framework of homogenization-based self-consistent formulations, in the viscoplastic, thermo-elastic and elasto-viscoplastic regimes. The project has significantly advanced Los Alamos' crystal plasticity models. The project introduced improvements in 3 different in-house codes ("VPSC," "TEPSCA," and "EVPSC") to be possibly implemented with future programmatic work.

Publications

Journal Articles

*Bennett, K. C., M. Zecevic, D. J. Luscher and R. A. Lebensohn. A thermo-elastoplastic self-consistent homogenization method for inter-granular plasticity with application to thermal ratcheting of TATB. 2020. *Advanced Modeling and Simulation in Engineering Sciences*. **7** (1): 3. (LA-UR-19-28919 DOI: 10.1186/s40323-019-0139-6)

*Bennett, K. C. and D. J. Luscher. Effective Thermoelasticity of Polymer-Bonded Particle Composites with Imperfect Interfaces and Thermally Expansive Interphases. 2019. *Journal of Elasticity*. **136** (1): 55-85. (LA-UR-17-31014 DOI: 10.1007/s10659-018-9688-z)

*Berbenni, S., V. Taupin and R. A. Lebensohn. A fast Fourier transform-based mesoscale field dislocation mechanics study of grain size effects and reversible plasticity in polycrystals. 2020. *Journal of the Mechanics and Physics of Solids*. **135**: 103808. (LA-UR-19-31410 DOI: 10.1016/j.jmps.2019.103808)

*Despr\xc3\xa9s, A., M. Zecevic, R. A. Lebensohn, J. D. Mithieux, F. Chassagne and C. W. Sinclair. Contribution of intragranular misorientations to the cold rolling textures of ferritic stainless steels. 2020. *Acta Materialia*. **182**: 184-196. (LA-UR-19-31386 DOI: 10.1016/j.actamat.2019.10.023)

*Gen\xc3\xa9e, J., S. Berbenni, N. Gey, R. A. Lebensohn and F. Bonnet. Particle interspacing effects on the mechanical behavior of a Fe–TiB2 metal matrix composite using FFT-based mesoscopic field dislocation mechanics. 2020. *Advanced Modeling and Simulation in Engineering Sciences*. **7** (1): 6. (LA-UR-19-31404 DOI: 10.1186/s40323-020-0141-z)

Lebensohn, R. A. Polycrystal plasticity models based on Green's functions: mean-field self-consistent and full-field Fast Fourier Transform formulations. *Handbook of Materials Modeling*. 1-27. (LA-UR-17-31125 DOI: 10.1007/978-3-319-42913-7_15-1)

*Lebensohn, R. A. and A. D. Rollett. Spectral methods for full-field micromechanical modelling of polycrystalline materials. 2020. *Computational Materials Science*. **173**: 109336. (LA-UR-18-28795 DOI: 10.1016/j.commatsci.2019.109336)

*Lieou, C. K. and C. A. Bronkhorst. Thermodynamic theory of crystal plasticity: Formulation and application to polycrystal fcc copper. 2020. *Journal of the Mechanics and Physics of Solids*. **138**: 103905. (LA-UR-19-31861 DOI: 10.1016/j.jmps.2020.103905)

*Liu, P. W., Z. Wang, Y. H. Xiao, R. A. Lebensohn, Y. C. Liu, M. F. Horstemeyer, X. Y. Cui and L. Chen. Integration of phase-field model and crystal plasticity for the prediction of process-structure-property relation of additively manufactured metallic materials. 2020. *International Journal of Plasticity*. **128**: 102670. (LA-UR-19-31422 DOI: 10.1016/j.ijplas.2020.102670)

*Messner, M. C., R. A. Lebensohn, E. Zepeda-Alarcon and N. R. Barton. A method for including diffusive effects in texture evolution. 2019. *Journal of the Mechanics and Physics of Solids*. **125**: 785-804. (LA-UR-18-23915 DOI: 10.1016/j.jmps.2019.01.016)

*Nagra, J. S., A. Brahme, J. Levesque, R. Mishra, R. A. Lebensohn and K. Inal. A new micromechanics based full field numerical framework to simulate the effects of dynamic recrystallization on the formability of HCP metals. 2020. *International Journal of Plasticity*. **125**: 210-234. (LA-UR-19-31405 DOI: 10.1016/j.ijplas.2019.09.011)

*Ran, H., T. de Riese, M. Llorens, M. A. Finch, L. A. Evans, E. Gomez-Rivas, A. Griera, M. W. Jessell, R. A. Lebensohn, S. Piazolo and P. D. Bons. Time for anisotropy: The significance of mechanical anisotropy for the development of deformation structures. 2019. *Journal of Structural Geology*. **125**: 41-47. (LA-UR-18-23499 DOI: 10.1016/j.jsg.2018.04.019)

*Segurado, J., R. A. Lebensohn and J. LLorca. Computational Homogenization of Polycrystals. *Advances in Applied Mathematics*. **51**: 1-114. (LA-UR-18-23540 DOI: 10.1016/bs.aams.2018.07.001)

Tome, C. and R. A. Lebensohn. Polycrystal Thermo-Elasticity Revisited: Theory and Applications. Submitted to *Comptes Rendus Mecanique*. (LA-UR-20-23936)

Zecevic, M., K. Bennett, D. J. Luscher and R. A. Lebensohn. New self-consistent homogenization for thermo-elastic polycrystals with imperfect interfaces. 2020. *Mechanics of Materials*. 103651. (LA-UR-20-24726 DOI: 10.1016/j.mechmat.2020.103651)

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*Zecevic, M., R. A. Lebensohn, R. J. McCabe and M. Knezevic. Modeling of intragranular misorientation and grain fragmentation in polycrystalline materials using the viscoplastic self-consistent formulation. 2018. *International Journal of Plasticity*. **109**: 193-211. (LA-UR-18-23679 DOI: 10.1016/j.ijplas.2018.06.004)

*Zecevic, M., R. A. Lebensohn, R. J. McCabe and M. Knezevic. Modelling recrystallization textures driven by intragranular fluctuations implemented in the viscoplastic self-consistent formulation. 2019. *Acta Materialia*. **164**: 530-546. (LA-UR-18-27030 DOI: 10.1016/j.actamat.2018.11.002)

*Zecevic, M., W. Pantleon, R. A. Lebensohn, R. J. McCabe and M. Knezevic. Predicting intragranular misorientation distributions in polycrystalline metals using the viscoplastic self-consistent formulation. 2017. *Acta Materialia*. **140**: 398-410. (LA-UR-18-22506 DOI: 10.1016/j.actamat.2017.08.056)

Zecevic, M. and R. A. Lebensohn. New robust self-consistent homogenization schemes of elasto-viscoplastic polycrystals. 2020. *International Journal of Solids and Structures*. **202**: 434-453. (LA-UR-20-21794 DOI: 10.1016/j.ijsolstr.2020.05.032)

Presentation Slides

Alexandrov, B. Unsupervised phase mapping of X-ray diffraction data by nonnegative factorization integrated with custom clustering. Presented at *Computational Data Science Approaches for Materials Conference 2019*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23081)

Bennett, K. Micro-thermomechanical modeling of PBX 9502 & self-consistent homogenization. Presented at *Internal Cross-divisional Research Meeting*, Los Alamos, New Mexico, United States, 2019-11-19 - 2019-11-19. (LA-UR-19-31411)

Zecevic, M., R. A. Lebensohn, R. J. Mccabe and M. Knezevic. PREDICTIONS OF FIELD FLUCTUATIONS IN HETEROGENEOUS MATERIALS. Presented at *TMS2019*, San Antonio, Texas, United States, 2019-03-10 - 2019-03-14. (LA-UR-19-22231)

Zecevic, M. and R. A. Lebensohn. New Robust Self-Consistent Homogenization Schemes of Elasto-Viscoplastic Polycrystals. Presented at *TMS 2020 149th Annual Meeting and Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21848)

Quantum Dot Sunlight Collectors for Building-Integrated Photovoltaics

Victor Klimov
20190232ER

Project Description

The Department of Energy aims to reduce the energy consumption of buildings by 50% by 2030, identifying building-integrated photovoltaics (BIPV) as an important component of this ongoing effort. The proposed project directly addresses this goal by introducing a new solution to BIPV, which is based on inexpensive luminescent sunlight collectors or luminescent solar concentrators (LSCs) integrated into a building envelope as semitransparent solar windows and/or wall panels coupled to edge-installed photovoltaics (PVs). The key innovation in this project is designer semiconductor quantum dots that exhibit close-to-unity emission efficiencies at near-infrared energies, combined with specially tailored optical spectra that feature strong absorptance across the solar spectrum and virtually complete suppression of self-absorption at the emission wavelength. These nearly ideal characteristics, never previously realized with any other fluorophores, will enable large-area sunlight collectors with efficiencies approaching a theoretical limit. The quantum-dot LSC technology developed in this project will become one of the vital elements of ongoing efforts on the realization of net-zero energy consumption buildings.

Technical Outcomes

This project has successfully accomplished its primary objective, that is, the demonstration of feasibility of high-performance large-area luminescent solar concentrators (LSCs) based on engineered quantum dots (QDs). Further, the team has identified a new LSC figure of merit which allows for reliable prediction of LSC performance based on QD optical characteristics. The insights gained from the conducted studies along with the demonstration of record-high LSC efficiencies will stimulate further advances in luminescent sunlight collectors and their exploitation in practical solar-energy technologies.

Publications

Journal Articles

Du, J., R. Singh, I. Fedin, A. S. Fuhr and V. I. Klimov. Spectroscopic insights into high defect tolerance of Zn:CuInSe2 quantum-dot-sensitized solar cells. Submitted to *Nature Energy*. (LA-UR-19-29575)

*Fuhr, A., H. J. Yun, S. A. Crooker and V. I. Klimov. Spectroscopic and Magneto-Optical Signatures of Cu1+ and Cu2+ Defects in Copper Indium Sulfide Quantum Dots. 2020. *ACS Nano*. **14** (2): 2212-2223. (LA-UR-20-20156 DOI: 10.1021/acsnano.9b09181)

Klimov, V. I., J. Du, I. Fedin, R. Singh and A. Fuhr. Spectroscopic insights into high defect tolerance of Zn:CuInSe2 quantum-dot-sensitized solar cells. Submitted to *Nature Energy*. (LA-UR-20-20157)

Presentation Slides

Gungor, K., O. Erdem, B. Guzelturk, E. Unal, M. Sak, S. Gaponenko, S. Jun, E. Jang and H. V. Demir. Strongly Polarized Light Generation from Isotropic Colloidal Quantum Dots Coupled to Fano Resonances. Presented at *2019 MRS Spring Meeting & Exhibit*, Phoenix, Arizona, United States, 2019-04-22 - 2019-04-26. (LA-UR-19-22937)

Evaluating and Increasing the Reliability of Supercomputer and Autonomous Vehicles (Rosen Scholar)

Constantine Sinnis
20190499ER

Project Description

This research is focused on the reliability and efficiency of safety-critical computing platforms such as autonomous vehicles (AVs) and High Performance Computing (HPC). As HPC and AVs become more prevalent throughout the National Nuclear Security Administration and the nation, the need for resilience in these systems is ever increasing. Neutron upsets pose a unique and unavoidable threat to these systems. The development of mitigation strategies will increase the reliability and therefore the utility of such systems.

Technical Outcomes

This project measured neutron-induced error rate of devices and algorithms for autonomous vehicles (AVs) and High Performance Computing (HPC). Thanks to beam experiments at Los Alamos Neutron Science Center (LANSCE) and fault injection the team understood the fault model, identified the most likely resources for failure, and paved a path to predict the error rate of future frameworks. Additionally, they designed and validated efficient and effective solutions to detect errors before they impact system functionality.

Publications

Conference Papers

Rech, P., F. Fernandes dos Santos, M. Brandalero, P. Basso and M. Shafique. Efficient Duplication With Comparison Strategy for Mixed-Precision Architectures. Presented at *HPCA (The 26th IEEE International Symposium on High-Performance Computer Architecture)*. (San Diego, California, United States, 2020-02-22 - 2020-02-22). (LA-UR-19-28021)

Presentation Slides

Rech, P. Reliability in the Era of Autonomous Vehicles and Supercomputers. Presented at *The Physics and Theoretical Division Colloquium*, los alamos, New Mexico, United States, 2019-10-31 - 2019-10-31. (LA-UR-19-32383)

Rech, P., D. Oliveira and P. Navaux. Increasing the Efficiency and Efficacy of Selective-Hardening for Parallel Applications. Presented at *DFT (The 32nd IEEE Inter)national Symposium on Defect and Fault Tolerance in VLSI and Nanotechnology Systems)*, delft, Netherlands, 2019-10-03 - 2019-10-03. (LA-UR-19-29993)

Posters

Martins Basso, P., F. Fernandes dos Santos and P. Rech. Impact of Tensor Cores and Mixed-Precision on the Reliability of Matrix Multiplication in GPUs. Presented at *RADECS*, Montpellier, France, 2019-09-15 - 2019-09-20. (LA-UR-19-29987)

Plutonium Gas Dynamics Using Small Samples and Laser Ablation Techniques

Robert Chrien
20200628ER

Project Description

This study will probe the interaction of metal particles with hydrogen gas. Hydriding occurs when hydrogen accumulates in the spaces between metal atoms. This process changes the physical properties of plutonium metal, leading to embrittlement and a less functional material. This work will focus on uranium and cerium metals, and the techniques thus developed will be employed to study plutonium. Laser pulses will be used to create metal particles from thin metal targets. The metal particles will be created in hydrogen gas, and chemical species will be determined using spectroscopic techniques. The rate of hydriding and the chemical species formed are of importance to many aspects of Los Alamos National Laboratory's plutonium mission.

Technical Outcomes

This work successfully fabricated cerium metal films of several thicknesses, laser ablated the films, and measured the temperature and emission spectra of the plumes. It was demonstrated the emission spectrum indicates whether the cerium metal plume is atomized or consists of metal particles. The temperature of the cerium metal plume was less in hydrogen (H2) than in helium (He), indicating no hydriding, which is consistent with the measured temperatures that were above where hydriding would occur.

Publications

Reports

Chrien, R. E. and B. L. Scott. Plutonium gas dynamics using small samples and laser ablation techniques (U). Unpublished report. (LA-UR-21-20503)

Advancing Energetic Additive Manufacturing by Creating a New Class of Energetic Material

David Chavez
20200633ER

Project Description

The national security challenge this project addresses is the need for structural energetic materials with higher manufacturing precision and higher performance. The United States had a strong focus on the development of insensitive energetic materials but this focus is now shifting toward the urgent need for the development of high-performance energetic materials. The high level goal of this project is the development of energetic structural materials with unprecedented 3-Dimensional printing precision and explosive performance. The impact on Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions includes novel energetic outputs and efficient explosive component design with control over performance output features.

Technical Outcomes

Two novel energetic monomers were successfully synthesized and chemically characterized. These materials were prepared from the commercially available starting materials under simple and efficient reaction conditions to provide the corresponding desired compounds. These two materials were characterized to determine thermal stability using thermal analysis methods. The materials were also characterized chemically to confirm the chemical structures. Additionally, the materials were characterized to determine explosive sensitivity properties. Preliminary polymerization reactions were also performed.

In situ Characterization of Radiation-Induced Transport

Yongqiang Wang
20200641ER

Project Description

The evolution of materials under irradiation is driven by the enhanced transport of atoms during irradiation. To understand, predict, and ultimately design new materials destined for nuclear energy applications, it is imperative to understand the motion of these atoms. Currently, there are no probes to directly measure this transport during irradiation. We propose to combine electrochemical measurements with ion beam irradiations to develop a first-of-its-kind capability to directly measure the transport of atoms during irradiation. This capability will provide unprecedented insight into the dynamical behavior of these materials, directly probing properties that have, to date, only been inferred. It will provide critical data for validating and benchmarking models of these materials. It will have wide applicability, and thus should provide fundamental information about materials performance in harsh environments related to a range of situations, from nuclear energy to functional materials to national security applications. Because this is being developed as part of Los Alamos National Laboratory's Center for Integrated Nanotechnology, the new capability will be available for external users as well.

Technical Outcomes

An in-situ electrochemical impedance spectroscopy (EIS) capability has been developed at the Ion Beam Materials Laboratory. The capability consists of two parts: (1) a high temperature sample stage and temperature controller (up to 950 Celsius) with electrical feedthroughs for EIS electrodes, heater power, thermocouple, and other signals and (2) Gamrr Reference 600+ Potentistat/Galvanostat/Zero resistance ammeter (ZRA) impedance spectrometer. The proof of principle for the new capability was successfully demonstrated on yttrium stabilized zirconia (YSZ) target with 200 keV (thousand electron volts) helium (He) ion irradiation.

Two Level Systems by Design to Mitigate Decoherence in Superconducting Quantum Computers

Leonardo Civale
20200657ER

Project Description

We are at the dawn of the second quantum revolution, which will have huge impact in computing, communications and sensing technologies. A worldwide race for supremacy in this field is on. The United States government is implementing a strong Quantum Information Science agenda, through the National Quantum Initiative Act. Quantum computers (QC) already exist, their capability to solve some problems efficiently is established, but they still cannot surpass classical computers because they only contain a small number of qubits (the quantum analog of the bit). The main constraint for the scale-up and further development of QC is the decoherence arising from interactions with uncontrolled degrees of freedom. Mitigating QC decoherence is one of the main scientific and technological challenges of our time. Particularly detrimental are sources of decoherence associated with material disorder, called two-level systems (TLS), whose microscopic origin is unknown. This project will implement a novel approach that we call TLS by design, using particle irradiation and implantation to introduce material disorder (structural defects and doping) with an unsurpassed level of control, with the purpose of creating TLS. This will allow the project to establish quantitative "defect - TLS" correlations, a necessary step to devise strategies to mitigate them.

Technical Outcomes

This project designed and fabricated 2-Dimensional coplanar waveguide (CPW) and 3-Dimensional superconducting radio frequency (SRF) cavity niobium (Nb) superconducting resonators. The team measured resonance frequencies and quality (Q) factors at room temperature, and for CPW, down to ~1 Kelvin (K) and obtained the temperature and pressure dependence of Q. Below ~3 K, Q decreases as pressure decreases, as expected for two-level systems (TLS), confirming that we can observe them.

In Situ Methods to Inform Design of Additively Manufactured Lattice Structures

John Carpenter
20200679ER

Project Description

This project studies the process-structure-property relationships for additively manufactured titanium alloy engineered lattice structures with collaborators from the Israeli Atomic Energy Commission using already granted beam time at the Diamond Light Source in the United Kingdom (April 2020). Current engineering models for optimizing the design of engineered lattice structures begin to lose accuracy when ligament dimensions fall to 1 millimeter (mm) and below. Achieving ligament dimensions lower than 1 mm is required for achieving the densities needed for applications related to the National Nuclear Security Administration (NNSA) applications. This project plans to monitor the evolution of porous defects and strain in the ligaments in order to identify how particular defect structures lead to failure in these structures. The goal is to understand how to design individual struts within a lattice structure for repeatable and predictable mechanical behavior. Lattice materials are of interest to the NNSA for a variety of weapons-based applications but integration has been slowed because of a lack of fundamental understanding of process-structure-property relationships.

Technical Outcomes

Additive manufacturing (AM) can build ordered metal structures with reduced density, termed lattice structures (LS), that provide structural materials as strong as metals but as light as plastics. To take advantage of this strength/density combination, the structure-property relationships that govern LS need to be developed. Through in situ and ex situ measurements, the needed data was collected and used in simulations. The simulation efforts showed that surface roughness was key to accurate predictions of strength.

Publications

Journal Articles

Britt, C., C. J. Montgomery, M. J. Brand, J. S. Carpenter and A. M. Beese. Effect of Processing Parameters and Strut Dimensions on the Microstructures and Hardness of Stainless Steel 316L Lattice-Emulating Structures Made by Powder Bed Fusion. 2021. *Additive Manufacturing*. 101943. (LA-UR-20-29423 DOI: 10.1016/j.addma.2021.101943)

Brown, D. W., V. Anghel, L. Balogh, L. Ravkov, B. Clausen, N. S. Johnson, R. M. Martinez, D. Pagan, G. Rafailov, M. Strantza and E. Zepeda-Alarcon. Evolution of the Microstructure of Laser Powder Bed Fusion Ti64 During Post-Build Heat Treatment. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-21-22622)

Johnson, N. S., P. Vulimiri, A. To, X. Zhang, C. Brice, B. Kappes and A. Stebner. Machine Learning for Materials Developments in Metals Additive Manufacturing. Submitted to *Additive Manufacturing*. (LA-UR-20-23464)

Strantza, M., R. K. Ganeriwala, B. Clausen, T. Q. Phan, L. E. Levine, D. C. Pagan, J. Ruff, W. E. King, N. S. Johnson, R. M. Martinez, V. Anghel and D. W. Brown. Effect of the scanning strategy on the formation of residual stresses in additively manufactured Ti-6Al-4V. Submitted to *Additive Manufacture*. (LA-UR-20-26528)

Presentation Slides

Brown, D. W., J. S. Carpenter, B. Clausen, J. C. Cooley, J. Zhang, E. B. Watkins, J. S. Park and P. Kenesei. The Prospects For Using Diffraction Based Techniques To Monitor Microstructural Evolution Under Manufacturing Conditions. Presented at *In-situ sensing and process monitoring for NNSA relevant materials and processes*, Los Alamos, New Mexico, United States, 2020-08-25 - 2020-08-25. (LA-UR-20-26449)

Brown, D. W., M. Strantza, G. Rafailov, E. Zepeda-Alarcon and D. Pagan. In-Situ Heat Treatment of Additively Manufactured Ti-6Al-4V. Presented at *International Conference on Additive Manufacturing*, Orlando, Florida, United States, 2020-11-16 - 2020-11-19. (LA-UR-20-29134)

Carpenter, J. S. Enabling Science Based Qualification in Metal Additive Manufacturing. Presented at *Institute of Materials Science Summer Lecture Series*, Los Alamos, New Mexico, United States, 2020-06-25 - 2020-06-25. (LA-UR-20-24592)

Carpenter, J. S., D. W. Brown, B. Clausen, J. C. Cooley, M. Strantza, A. Losko, N. Johnson, J. Park, P. Kenesei and J. Almer. Using High Energy X-Ray Diffraction to Probe Additively Manufactured Metals Over a Range of Length and Time Scales. Presented at *TMS Annual Meeting*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-21594)

Carpenter, J. S., D. W. Brown, B. Clausen, J. C. Cooley, M. Strantza, A. Losko, N. Johnson, J. Park, P. Kenesei and J. Almer. Using High Energy X-Ray Diffraction to Probe Additively Manufactured Metals Over a Range of Length and Time Scales. Presented at *International Conference on Additive Manufacturing*, Orlando, Florida, United States, 2020-11-16 - 2020-11-16. (LA-UR-20-27536)

Ryder, M. A., C. J. Montgomery, M. J. Brand, R. M. Pacheco, J. S. Carpenter and D. A. Lados. Design of Additively Manufactured Steels for Fatigue-Critical Applications. Presented at *TMS Annual Meeting 2020*, San Diego, California, United States, 2020-02-24 - 2020-02-24. (LA-UR-20-21657)

Development of Improved High Temperature Fuel and Cladding Materials for Advanced Reactors

Stuart Maloy
20200692ER

Project Description

This research has a strong tie to multiple missions at the laboratory. Specifically, the research supports energy security for development of improved materials for nuclear reactor applications but the cladding material being developed also has applications in fossil energy, so it supports that area indirectly as well. This research will also provide new data on nuclear fuels. The research could provide new discoveries in the area of nuclear, particle, cosmology and astrophysics and a basic understanding in materials by studying radiation effects in this new innovative additively manufactured material. It is expected that this research will result in development of new improved nuclear fuels for advanced reactors including microreactors and fuel for nuclear thermal propulsion and advanced high temperature reactors. Initial research on the cladding material and fuel shows excellent high temperature properties pointing to excellent chance of success in this research.

Technical Outcomes

A significant outcome from the tri-carbide fuels work is developing the processing technique for oxide solutionization followed by carbo-thermic reduction. This outcome advanced the current processing knowledge and will impact the synthesis of future fuel material systems. The results fill a knowledge gap on the impact of irradiation on additively manufactured ferritic steels. These results will support proposals for neutron irradiations. The ion irradiation results will place Los Alamos in a position to support advanced reactor initiatives.

Publications

Journal Articles

Eftink, B. P., D. Vega, O. El Atwani, D. Sprouster, Y. S. Yoo, T. E. Steckley, E. Aydogan, C. M. Cady, M. Al-Sheikhly, T. J. Lienert and S. A. Maloy. Tensile properties and microstructure of additively manufactured Grade 91 steel for nuclear applications. 2020. *Journal of Nuclear Materials*. 152723. (LA-UR-20-25204 DOI: 10.1016/j.jnucmat.2020.152723)

Presentation Slides

Eftink, B. P., D. Vega, D. Sprouster, C. M. Cady, O. El Atwani, M. Al-Sheikhly, T. Lienert and S. A. Maloy. High Temperature Strength of Additively Manufactured Grade 91 steel. Presented at *TMS*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-21871)

Other

Eftink, B. P. Gr91 steel cavities data set. Dataset. (LA-UR-20-29007)

Detonator Powder Pressing Study

John Young
20200766ER

Project Description

The research and development goals of this project originate from a collaboration between Detonation Science and Technology and Detonator Production to develop a scientific understanding of current detonator powder pressing processes, to advance the manufacturing capabilities when pressing to a force, and to identify potential pressing effects, if any, on detonator performance and lifetimes. Current detonator manufacturing methods derive from performance-based experiments made in the 1940s, and do not draw from a modern scientific knowledge base. The proposed project 1) refines science-based knowledge and applications in detonator manufacturing, 2) demonstrates advanced diagnostics for physics-based performance data, and 3) adds to existing knowledge on detonator powder characteristics and detonator predictive lifetimes. The project aims to improve science and engineering understandings of powder pressing parameters and their potential effect(s) on detonator performance and lifetimes. Results will be of interest to other laboratories and broaden detonator design space in addition to advancing detonator manufacturing techniques and processes.

Technical Outcomes

Results suggest pressing to a force is a viable option. When pressing to a force the desired results are easier to achieve and require pressing fewer parts to accomplish the goal. During test fire there were no significant differences in the performance of the pressed cups.

Electronic Transport in Atomically Thin Materials at Far from Mechanical Equilibrium Conditions

Michael Pettes
20190516ECR

Project Description

Transition metal dichalcogenides (TMDs) are particularly sensitive to mechanical strain as they are capable of experiencing high strains without nucleating defects to release excess energy. As both the effective mass and optical phonon energies in these materials decrease with strain, and since the electron lifetime is inversely proportional to the phonon energy and occupation, an increase of electron mobility is hypothesized to occur with tensile elastic strain. This is significant as the drift velocity directly determines the switching speed in ultra-fast transistors as well as excitonic recombination dynamics in nano photonic devices. This research will address the fundamental question of how the variable of strain influences electronic performance in 2-dimensional materials, so that it can be fully accounted for in the design of next-generation nano electronic devices. Upon completion of this project, the PI will have established a globally unique in situ TEM-based structure-property characterization capability to quantify and correlate atomic-level strain experienced by a suspended nano material with electronic transport properties, a technique currently not possible and very relevant to structure-processing-property testing of other thin films including actinide-based materials required for advanced weapons and sensor applications.

Publications

Journal Articles

Pettes, M. T., A. Londono Calderon, D. J. Williams, B. H. Savitzky, C. Ophus, S. Ma and H. Zhu. Evidence of Intrinsic Helical Twist and Chirality in Ultrathin Tellurium Nanowires. Submitted to *Advanced Functional Materials*. (LA-UR-21-21904)

Pettes, M. T., A. Londono Calderon, D. J. Williams, C. Ophus, B. Savitsky and M. M. Schneider. Local Lattice Deformation of Tellurene Grain Boundaries by Four-Dimensional Electron Microscopy. 2021. *The Journal of Physical Chemistry C*. **125** (6): 3396-3405. (LA-UR-20-27603 DOI: 10.1021/acs.jpcc.1c00308)

Pettes, M. T., A. Londono Calderon, D. J. Williams and C. Ophus. 1D to 2D Transition in Tellurium Observed by 4D Electron Microscopy. 2020. *Small*. **16** (49): 2005447. (LA-UR-20-25292 DOI: 10.1002/smll.202005447)

*Wei, W., C. K. Dass, J. R. Hendrickson, R. D. Montano, R. E. Fischer, Z. Xiaotian, T. H. Choudhury, J. M. Redwing, W. Yongqiang and M. T. Pettes. Locally defined quantum emission from epitaxial few-layer tungsten diselenide. 2019. *Applied Physics Letters*. **114** (21): 213102. (LA-UR-18-27142 DOI: 10.1063/1.5091779)

*Yazdani, S., R. Kashfi-Sadabad, M. D. Morales-Acosta, R. D. Montano, N. V. Tuoc, D. T. Huan, M. Zhou, Y. Liu, J. He and M. T. Pettes. Thermal transport in phase-stabilized lithium zirconate phosphates. 2020. *Applied Physics Letters*. **117** (1): 11903. (LA-UR-20-24103 DOI: 10.1063/5.0013716)

Presentation Slides

Londono Calderon, A., C. Ophus, D. J. Williams and M. T. Pettes. Quantifying peak profile analysis of 2D Tellurium nanostructures by 4D-STEM. Presented at *2020 virtual MRS Spring/Fall meeting & exhibit*, Los Alamos, New Mexico, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-29012)

Londono Calderon, A., D. J. Williams, B. H. Savitzky and M. T. Pettes. Towards Crystallographic Orientation and Strain Mapping of 1D & 2D Tellurium from 4D-STEM. Presented at *Microscopy & Microanalysis 2020 virtual meeting*, Los Alamos, New Mexico, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-25117)

Pettes, M. T. Deterministic Defect Emission from Epitaxial TMD Thin Films. Presented at *Invited Seminar at 2D Crystal Consortium-Materials Innovation Platform NSF Site Visit Year 4*, University Park, Pennsylvania, United States, 2019-05-21 - 2019-05-21. (LA-UR-19-24535)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited seminar at University of California, Merced Mechanical Engineering Department*, Merced, California, United States, 2019-09-27 - 2019-09-27. (LA-UR-19-29644)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited Seminar at North Carolina*

State University Mechanical Engineering Department, Raleigh, North Carolina, United States, 2019-10-18 - 2019-10-18. (LA-UR-19-30501)

Pettes, M. T. Deterministic Quantum Emission in an Epitaxial 2D Material. . (LA-UR-19-25907)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited Seminar at Yale University Energy Sciences Institute*, New Haven, Connecticut, United States, 2019-07-30 - 2019-07-30. (LA-UR-19-27328)

Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials: WSe2 and Te. Presented at *Invited Seminar at Rice University Materials Science Department*, Houston, Texas, United States, 2020-01-16 - 2020-01-16. (LA-UR-20-20408)

Pettes, M. T. Emergent Phenomena in van der Waals Materials: Advancements in Characterization. Presented at *Invited Seminar presented to the University of Minnesota*, Minneapolis (online), Minnesota, United States, 2020-10-28 - 2020-10-28. (LA-UR-20-28618)

Posters

Londono Calderon, A., D. J. Williams and M. T. Pettes. Strain mapping of grain boundary in two-dimensional tellurene by 4D-STEM. Presented at *2020 CINT Annual Meeting*, Online, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27301)

Pettes, M. T. Intrinsic and Extrinsic Control over Physical Properties in a Representative Atomically Thin Semiconductor. Presented at *2019 National Academy of Engineering EU-US Frontiers of Engineering symposium*, Stockholm, Sweden, 2019-11-18 - 2019-11-20. (LA-UR-19-31073)

Pettes, M. T., A. Londono Calderon and D. J. Williams. Crystallographic Orientation of 1D & 2D Tellurium from 4D Scanning Transmission Electron Microscopy. Presented at *13th Annual Postdoctoral Technical Showcase, Sandia National Laboratories*, Albuquerque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-32519)

Adaptive Framework for Enabling Real-time Feedback During Three-dimensional Mesoscale Microstructure Evolution Measurements

Reeju Pokharel
20190571ECR

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.

Publications

Journal Articles

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)

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. 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)

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)

Nonlinear Photonics of Topological Phase Transitions in the Graphene Family

Wilton Junior de Melo Kort-Kamp
20190574ECR

Project Description

Topology studies the properties of space that are preserved under continuous deformations. Distinct topologies are mathematically characterized by integers called topological invariants; topologically equivalent objects, such as a donut and a coffee cup, share the same invariant (the number of “holes”). An object undergoes a topological phase transition whenever an abrupt transformation changes the topological invariant. Over the past few decades, notions of topology have become ubiquitous in materials science, culminating in the 2016 Nobel Prizes in Physics and Chemistry. The topological nature of electronic states is a pivotal concept in various recent advances in low dimensional quantum systems. This project aims to investigate ultrafast nonlinear photonic phenomena in newly discovered two-dimensional materials of the graphene family supporting topological phase transitions. The project focuses on discovery and application of fundamental material properties for controlled functionality and performance prediction beyond the linear response regime, and it will significantly advance the country’s initiatives in nanotechnology and nanophotonics. Investigations on the interplay between topological chiral edge states and nonreciprocal behavior arising from nonlinearities will unveil the potential of the graphene family materials as a reliable platform for information transport, with implications for quantum computing.

Publications

Journal Articles

Caravelli, F., A. Hamma, S. Oliviero and L. Leone. Random Matrix Theory of the Isospectral twirling. Submitted to *SciPost Physics*. (LA-UR-20-30225)

Caravelli, F., B. Yan, L. Garcia-Pinto and A. Hamma. Energy storage and coherence bounds in closed and open quantum batteries. Submitted to *Quantum*. (LA-UR-20-30512)

de Melo Kort-Kamp, W. J., F. Culchac, F. Rosa, C. Farina, R. Capaz and F. Pinheiro. Harnessing the photonic local density of states in graphene Moir\xc3\xa9 superlattices. Submitted to *PRB*. (LA-UR-21-20508)

Malla, R. K., V. Y. Chernyak and N. Sinitsyn. Nonadiabatic transitions in Landau-Zener grids: integrability and semiclassical theory. Submitted to *Physical Review B*. (LA-UR-21-20136)

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear photonics of topological Dirac fermions in spin-orbit coupled graphene family materials. Submitted to *Communications physics*. (LA-UR-20-30407)

Muniz, Y., A. Manjavacas, C. Farina, D. A. R. Dalvit and W. J. de Melo Kort-Kamp. Unraveling the decay mechanisms of two-quanta spontaneous photonic transitions. Submitted to *Nature Photonics*. (LA-UR-20-20456)

Muniz, Y., C. Farina and W. J. de Melo Kort-Kamp. Casimir forces in the flatland: impact of topological phase transitions and quantum Hall physics. Submitted to *Physical Review B*. (LA-UR-20-28079)

Presentation Slides

Malla, R. K., A. B. Saxena and W. J. de Melo Kort-Kamp. Nonlinear planar Hall effect in graphene family monolayers. Presented at *APS March meeting, 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22394)

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear optical response of graphene family materials near topological phase transitions. Presented at *2020 APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21863)

Plutonium Defect Characterization through Mechanical Deformation

Taylor Jacobs
20200557ECR

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.

Publications

Presentation Slides

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)

The Role of Defects in Mechanical Instabilities of Additively Manufactured Lattice Materials

Rachel Collino
20200588ECR

Project Description

3-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.

Excited State Dynamics for Spin Systems

Tammie Nelson
20180552ECR

Project Description

This project will use and develop nonadiabatic excited state molecular dynamics, a software package acknowledged by NNSA for open source, to provide novel computational capabilities critical for understanding light-induced dynamics in many technologically relevant materials. The developed capabilities will have extremely broad applications relevant to the current and future Laboratory/DOE missions, particularly benefitting the primary goal of the Materials for the Future focus area and in the future modeling of materials important for the Laboratory core mission, such as explosives. The project will develop a new computational capability that can be applied to advance modeling of photostability and photodegradation, and spin-crossover induced sensitivity changes in new classes of explosive materials. The high level goals of the project are to develop a modeling capability to describe the spin dynamics in realistic materials and to apply the capability for the prediction, control and design of specific material properties.

Technical Outcomes

The project resulted in extension of excited-state nonadiabatic molecule dynamics (NAMD) capability for open-shell systems implemented in the NEXMD software. We developed the spin-unrestricted CIS and TD-SCF formalisms for the ground and excited states, analytical derivatives, and nonadiabatic derivative couplings for the respective potential energy surfaces. The new capability has been demonstrated in simulations of photoinduced bond breaking reactions of several molecular systems.

Publications

Journal Articles

Freixas, V. M., A. J. White, T. R. Nelson, H. Song, D. V. Makhov, D. Shalashilin, S. Fernandez-Alberti and S. Tretiak. Non-Adiabatic Excited State Molecular Dynamics Methodologies: comparison and convergence. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-20549)

*Lystrom, L., Y. Zhang, S. Tretiak and T. Nelson. Site-Specific Photodecomposition in Conjugated Energetic Materials. 2018. *The Journal of Physical Chemistry A*. **122** (29): 6055-6061. (LA-UR-18-24161 DOI: 10.1021/acs.jpca.8b04381)

Nelson, T. R., A. J. White, J. A. Bjorgaard, A. E. Sifain, Y. Zhang, B. T. Nebgen, S. Fernandez-Alberti, D. V. Mozyrsky, S. Tretiak and A. E. Roitberg. Non-adiabatic Excited State Molecular Dynamics: theory and applications for modeling photophysics in extended molecular materials. Submitted to *Chemical Reviews*. (LA-UR-19-25569)

Nelson, T. R., B. T. Nebgen, A. J. White, Y. Zhang, H. Song, J. A. Bjorgaard, A. E. Sifain, B. Rodriguez-Hernandez, V. M. Freixas, S. Fernandez-Alberti, A. Roitberg, W. F. I. Malone and S. Tretiak. NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22362)

*Nelson, T. R., D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. F. Galindo, V. D. Kleiman, S. Fernandez-Alberti, A. E. Roitberg and S. Tretiak. Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. 2018. *Nature Communications*. **9** (1): 2316. (LA-UR-17-30143 DOI: 10.1038/s41467-018-04694-8)

Nelson, T. R., S. Tretiak, D. O. Alvarez, S. Fernandez-Alberti and J. M. Lupton. Let Digons be Bygones: The Fate of Excitons in Curved pi-systems. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-18-29242)

Nelson, T. R., V. M. Freixas, D. Ondarse-Alvarez, P. Nijjar, A. Mikhailovsky, C. Zhou, S. Fernandez-Alberti, G. C. Bazan and S. Tretiak. Experimental and Theoretical Study of Energy Transfer in a Chromophore Triad: What Makes Modeling Dynamics Successful?. Submitted to *Journal of Chemical Physics*. (LA-UR-20-23551)

*Nelson, T., S. Fernandez-Alberti, A. E. Roitberg and S. Tretiak. Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. 2017. *The Journal of Physical Chemistry Letters*. **8** (13): 3020-3031. (LA-UR-17-23765 DOI: 10.1021/acs.jpclett.7b00790)

Rodriguez-Hernandez, B., T. R. Nelson, N. Oldani, A. Martinez-Mesa, L. Uranga-Pina, Y. Segawa, S. Tretiak, K. Itami and S. Fernandez-Alberti. Exciton spatial dynamics and self-trapping in carbon nanocages. Submitted to *Journal of Physical Chemistry A*. (LA-UR-20-29357)

Sifain, A. E., B. J. Gifford, L. A. Lystrom, D. W. Gao, T. R. Nelson and S. Tretiak. NEXMD Modeling of Photoisomerization Dynamics of 4-Styrylquinoline. Submitted to *Journal of Physical Chemistry A*. (LA-UR-18-28405)

*Zhang, Y., T. Nelson and S. Tretiak. Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. 2019. *Journal of Chemical Theory and Computation*. **151** (15): 154109. (LA-UR-19-24300 DOI: 10.1063/1.5116550)

*Zhang, Y., T. R. Nelson and S. Tretiak. Nonadiabatic Excited-State Molecular Dynamics for Open-Shell Systems. 2020. *Journal of Chemical Theory and Computation*. **16** (4): 2053-2064. (LA-UR-19-29917 DOI: 10.1021/acs.jctc.9b00928)

Reports

Nelson, T. R. Excited State Dynamics for Spin Systems. Unpublished report. (LA-UR-18-25372)

Zhang, Y. Non-adiabatic Excited State Molecular Dynamics Modeling of Photochemistry and Polariton Chemistry. Unpublished report. (LA-UR-21-20629)

Presentation Slides

Nelson, T. R. 20180552ECR: Excited State Dynamics for Spin Systems. . (LA-UR-19-28487)

Zhang, Y. Non-adiabatic Excited State Molecular Dynamics Modeling of Photochemistry and Polariton Chemistry. . (LA-UR-21-20630)

Hybrid Density Functional Theory

Travis Sjostrom
20180613ECR

Project Description

This proposal is primarily motivated by a pressing need to understand and predict the basic properties of matter in the so-called warm dense matter regime. Under these extreme conditions materials properties are often difficult to measure and manipulate in well-controlled experiments and a reliable theoretical support is needed. These properties, such as the equation of state and transport properties, are critical for modeling in astrophysics, inertial confinement fusion, and weapons physics, making the ability to simulate and predict materials properties of particular importance. Our approach does not lead to the prohibitive computational scaling cost of the conventional numerical implementations, and is amenable to temperatures and pressures that are presently inaccessible by current approaches. Los Alamos has a prime interest in the materials properties of warm dense matter in terms of application to various programs. This will be the first ab initio method to bridge ambient to plasma conditions and will significantly enhance the theoretical characterization of high-energy density materials and matter in extreme conditions.

Technical Outcomes

This project developed a new theory and computational methods for hybrid density functional theory. This code implementation was made in the Quantum-espresso program, which required significant development to make the program amenable to very high temperatures and make use of orbital-free functionals. The code was benchmarked using very computationally expensive standard density functional theory approaches on high performance computers. This project has resulted in a functional version of the code now being used for equation of state calculations for extreme conditions.

Publications

Presentation Slides

Hollebon, P. J. and T. Sjostrom. High temperatures Density Functional Theory Calculations. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-22002)

Sjostrom, T. Hybrid Density Functional Theory: Combining Kohn-Sham and orbital-free DFT. Presented at *CECAM: Fundamentals of Density Functional Theory for T> 0 : Quantum meets Classical*, Lausanne, Switzerland, 2019-05-20 - 2019-05-23. (LA-UR-19-24617)

Probing Quantum Fluctuations via Thermal Expansion Measurements under Pressure

Priscila Rosa
20180618ECR

Project Description

This project will investigate quantum fluctuations by the development of thermal expansion measurements under pressure. This theme directly addresses the Laboratory's vision of Materials for the Future by providing the science required to discover, understand and ultimately control complex and collective forms of matter. As outlined in the Department of Energy (DOE)/Basic Energy Sciences (BES) Basic Research Needs report, quantum matter specifically is the next frontier for realizing this vision and has exceptional potential to revolutionize energy relevant technologies. Not only addressing a fundamental problem of immediate scientific importance that underlies an ability to anticipate new quantum states, this project also develops a new capability of thermal expansion measurements under extreme conditions that will enable understanding and control of new materials and new physics that may emerge in the future.

Technical Outcomes

This project succeeded in its major goal of developing a new experimental capability that allows the use of optical fibers under applied pressure to measure the thermal expansion and magnetostriction of materials of interest. This capability, combined with other thermodynamic and transport probes under applied pressure, provides a powerful toolkit for the investigation of a variety of phase transitions and complex phases from superconducting transition in strongly correlated materials to the phase stability of plutonium.

Publications

Journal Articles

*Piva, M. M., S. M. Thomas, Z. Fisk, J. -. X. Zhu, J. D. Thompson, P. G. Pagliuso and P. F. S. Rosa. Putative hybridization gap in CaMn2Bi2 under applied pressure. 2019. *Physical Review B*. **100** (4): 045108. (LA-UR-19-28476 DOI: 10.1103/PhysRevB.100.045108)

*Robinson, P. J., J. Munarriz, M. E. Valentine, A. Granmoe, N. Drichko, J. R. Chamorro, P. F. Rosa, T. M. McQueen and A. N. Alexandrova. Dynamical Bonding Driving Mixed Valency in a Metal Boride. 2020. *Nature Materials*. **59** (27): 10996-11002. (LA-UR-19-30421 DOI: 10.1002/anie.202000945)

*S. Rosa, P. F., S. M. Thomas, F. F. Balakirev, E. D. Bauer, R. M. Fernandes, J. D. Thompson, F. Ronning and M. Jaime. Enhanced Hybridization Sets the Stage for Electronic Nematicity in CeRhIn5. 2019. *Physical Review Letters*. **122** (1): 016402. (LA-UR-18-30371 DOI: 10.1103/PhysRevLett.122.016402)

Overdriven Shock and Initiation Effects on Detonator-Scale Energetic Materials

Kathryn Brown
20180633ECR

Project Description

One of the missions of Los Alamos National Laboratory is the development of new primary detonators for our nuclear stockpile. Research and development of new detonators is costly and time-consuming, and relevant physics data, including velocity and shock wave propagation, on the detonator scale is currently unavailable to the scientists that model old and new detonators. This project seeks to develop a rapid throughput detonator test bed by using a laser-driven configuration rather than an electrically-driven configuration. The use of high-speed imaging diagnostics will characterize explosive material that has been overdriven to detonation.

Technical Outcomes

A laser driven flyer plate testbed for detonator development was built and tested in performance. High speed imaging of the flyer geometry as a function of flight time and laser drive energy were acquired for system characterization. The system was demonstrated to initiate detonation in the Department of Energy (DOE) detonator explosive. Initial experiments to shape the flyer to generate convergent shocks were performed.

Publications

Journal Articles

Brown, K. E., K. J. Ramos and S. D. Mcgrane. Considerations for Ultrafast Spectroscopy on Shocked Explosives: Preliminary Investigations into using the Explosive as Impactor. Submitted to *Proceedings of the 2018 International Detonation Symposium*. (LA-UR-18-29489)

Conference Papers

Brown, K. E., K. J. Ramos and S. D. Mcgrane. Considerations for Ultrafast Spectroscopy on Shocked Explosives: Preliminary Investigations into using the Explosive as Impactor. Presented at *16th International Detonation Symposium*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-15). (LA-UR-18-25798)

Reports

Brunell, A. Internship After Action Review (AAR). Unpublished report. (LA-UR-18-26605)

Brunell, A. Internship Review Essay. Unpublished report. (LA-UR-18-26606)

Presentation Slides

Brown, K. E. Picosecond to Nanosecond Spectroscopy of Shocked Reactive Materials. Presented at *Seminars at Cornell and Coe Colleges*, Mount Vernon, Iowa, United States, 2019-02-21 - 2019-02-21. (LA-UR-19-21400)

Brown, K. E. Probing the Chemistry of Shocked Energetic Materials at Picosecond to Nanosecond Timescales. Presented at *Invited seminar at University of Missouri*, Columbia, Missouri, United States, 2019-09-27 - 2019-09-27. (LA-UR-19-29634)

Moore, D. S. Dynamic compression induced chemistry. Presented at *Dynamic Compression Summer School*, Chicago, Illinois, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-26654)

Conformal Field Theories with the Bootstrap

Emil Mottola
20180709PRD1

Project Description

The ultimate goal of this project is to help the development of new materials with properties suitable for applications in high-performance electrical circuits and quantum computing. This pursuit is extremely relevant for national security, for it holds the promise of significant technological and computational advances. Through the theoretical study of newly discovered critical theories with promising properties, the project aims to provide a solid framework for further theoretical developments, and to guide the experimental effort for the development of new materials.

Publications

Journal Articles

Henriksson, J., S. R. Kousvos and A. Stergiou. Analytic and Numerical Bootstrap of CFTs with O(m) \xc3\x97 O(n) Global Symmetry in 3D. Submitted to *SciPost Physics*. (LA-UR-20-23147)

Henriksson, J. and A. Stergiou. Perturbative and Nonperturbative Studies of CFTs with MN Global Symmetry. Submitted to *Scipost*. (LA-UR-21-20310)

*Kousvos, S. and A. Stergiou. Bootstrapping mixed correlators in three-dimensional cubic theories II. 2020. *SciPost*. **8** (6): 085. (LA-UR-19-30978 DOI: 10.21468/SciPostPhys.8.6.085)

*Lin, Y., D. Meltzer, S. Shao and A. Stergiou. Bounds on Triangle Anomalies in (3+1)d. 2020. *Physical Review D*. **101** (12): 125007. (LA-UR-19-30323 DOI: 10.1103/PhysRevD.101.125007)

*Manenti, A., A. Vichi and A. Stergiou. Implications of ANEC for SCFTs in four dimensions. 2020. *Journal of High Energy Physics*. **2020** (1): 93. (LA-UR-19-25902 DOI: 10.1007/JHEP01(2020)093)

Mottola, E., A. Sadofyev and A. Stergiou. Effective Field Theory and Axions in Weyl Semimetals. Submitted to *Physical Review Letters*. (LA-UR-21-20979)

Osborn, H. and A. Stergiou. Heavy Handed Quest for Fixed Points in Multiple Coupling Scalar Theories in the \xce\xb5 Expansion. Submitted to *Journal of High Energy Physics*. (LA-UR-20-27569)

*Stergiou, A. Bootstrapping MN and tetragonal CFTs in three dimensions. 2019. *SciPost Physics*. **7** (1): 010. (LA-UR-19-25903 DOI: 10.21468/SciPostPhys.7.1.010)

*Stergiou, A. and S. Kousvos. Bootstrapping mixed correlators in three-dimensional cubic theories. 2019. *SciPost Physics*. **6** (3): 035. (LA-UR-19-25906 DOI: 10.21468/SciPostPhys.6.3.035)

*Stergiou, A. and S. Rychkov. General properties of multiscalar RG Flows in d=4−\xce\xb5. 2019. *SciPost Physics*. **6** (1): 008. (LA-UR-19-25904 DOI: 10.21468/SciPostPhys.6.1.008)

Presentation Slides

Stergiou, A. Uncovering the Structure of the \xce\xb5 Expansion. Presented at *University of Crete HEP Seminars*, Heraklion, Greece, 2020-10-06 - 2020-10-06. (LA-UR-20-27835)

Stergiou, A. Conformal Bootstrap and Continuous Phase Transitions in 3D. Presented at *ERG 2020*, Kyoto, Japan, 2020-11-02 - 2020-11-06. (LA-UR-20-28986)

Stergiou, A. Conformal Bootstrap and Critical Phenomena. Presented at *LANL P/T Colloquium*, Los Alamos, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20104)

Stergiou, A. Strongly-coupled Physics Through a Conformal Field Theory Lens (IC project w20_strongcftlens). . (LA-UR-21-21777)

Exploration of New Topological States of Matter in Strongly Correlated Materials and in Ultra-high Magnetic Fields

Neil Harrison
20180713PRD2

Project Description

The use of the world-unique 100 Tesla (T) capability at the Los Alamos National High Magnetic Field Laboratory (NHMFL) and f-electron materials to search for novel topological phases will open up a new field of research on topology in strongly correlated matter. Topology is seen as a promising route for the development of new electronics and quantum computation, and it is therefore in the national interest to develop the highest quality materials. It is anticipated that several entirely new regimes of physics will emerge in very strong magnetic fields. This project will help establish Los Alamos as a world-leader in topology at extremely high magnetic field and in topological materials with strong electronic correlations.

Publications

Journal Articles

*Boschini, F., D. Bugini, M. Zonno, M. Michiardi, R. P. Day, E. Razzoli, B. Zwartsenberg, M. Schneider, E. H. Da Silva Neto, S. Dal Conte, S. K. Kushwaha, R. J. Cava, S. Zhdanovich, A. K. Mills, G. Levy, E. Carpene, C. Dallera, C. Giannetti, D. J. Jones, G. Cerullo and A. Damascelli. Role of matrix elements in the time-resolved photoemission signal. 2020. *Physical Review B*. **22** (2): 23031. (LA-UR-18-30021 DOI: 10.1088/1367-2630/ab6eb1)

*Cai, S., J. Guo, V. A. Sidorov, Y. Zhou, H. Wang, G. Lin, X. Li, Y. Li, K. Yang, A. Li, Q. Wu, J. Hu, S. K. Kushwaha, R. J. Cava and L. Sun. Independence of topological surface state and bulk conductance in three-dimensional topological insulators. 2018. *npj Quantum Materials*. **3** (1): 62. (LA-UR-19-26035 DOI: 10.1038/s41535-018-0134-z)

*Cai, S., S. K. Kushwaha, J. Guo, V. A. Sidorov, C. Le, Y. Zhou, H. Wang, G. Lin, X. Li, Y. Li, K. Yang, A. Li, Q. Wu, J. Hu, R. J. Cava and L. Sun. Universal superconductivity phase diagram for pressurized tetradymite topological insulators. 2018. *Physical Review Materials*. **2** (11): 114203. (LA-UR-19-26036 DOI: 10.1103/PhysRevMaterials.2.114203)

*Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Physical Review X*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

*Rosa, P., Y. Xu, M. Rahn, J. Souza, S. Kushwaha, L. Veiga, A. Bombardi, S. Thomas, M. Janoschek, E. Bauer, M. Chan, Z. Wang, J. Thompson, N. Harrison, P. Pagliuso, A. Bernevig and F. Ronning. Colossal magnetoresistance in a nonsymmorphic antiferromagnetic insulator. 2020. *npj Quantum Materials*. **5** (1): 52. (LA-UR-20-20098 DOI: 10.1038/s41535-020-00256-8)

Presentation Slides

Kushwaha, S. K. Development and study of the novel topological quantum materials. Presented at *Invited Colloquium*, Kalamazoo, Michigan, United States, 2020-03-16 - 2020-03-17. (LA-UR-20-22457)

Kushwaha, S. K. Development and study of novel topological materials. Presented at *Interview presentation*, Houston, Texas, United States, 2020-07-29 - 2020-07-29. (LA-UR-20-25748)

Kushwaha, S. K., M. K. Chan, N. Harrison, P. Ferrari Silveira Rosa, S. M. Thomas, E. D. Bauer, F. Ronning, J. Park and J. D. Thompson. Magnetic field induced Fermi liquid in a candidate topological Kondo insulator. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22244)

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, E. D. Bauer, J. D. Thompson, J. Zhu, C. Cao, F. Ronning and N. Harrison. Insulator/metal transition in a Topological Kondo Insulator at 60 T. Presented at *NSF meeting*, Tallahassee, Florida, United States, 2018-11-14 - 2018-11-14. (LA-UR-18-30652)

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, E. D. Bauer, J. D. Thompson, J. Zhu, F. Ronning, N. Harrison and C. Chao. Transport and magnetic properties of correlated Ce3Bi4Pd3 at high magnetic fields. Presented at *APS March Meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-08. (LA-UR-19-23573)

Kushwaha, S. K., M. K. Chan, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa, N. Harrison and J. Park. Metallization and Fermi-liquid state in a Kondo-insulator in high magnetic fields. Presented at

Dynamic Quantum Matter and Materials, Jacksonville, Florida, United States, 2020-12-14 - 2020-12-16. (LA-UR-20-30245)

Posters

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning and N. Harrison. Field induced metallic state in Ce3Bi4Pd3 Correlated Kondo material. Presented at *CNLS 39th Annual Conference - Strongly Correlated Quantum Materials*, Santa Fe, New Mexico, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-23792)

Development of an Innovative Mechanical Testing System and Techniques for Characterizing Irradiated Advanced Cladding Concepts and Novel Materials

Jonathan Gigax
20180744PRD3

Project Description

The goal of this project is to develop a novel in situ mechanical testing devices to perform analysis on specimen volumes on the microscale and approaching the macroscale. The device (commercially unavailable) will integrate high temperature and high strain rate capabilities to probe the mechanical response under extreme conditions. Macroscale mechanical testing of neutron irradiated materials has been used extensively to understand mechanical property (tensile, ductility, creep, hardness) changes after irradiation. Such testing is critical to the continued safe operation of the nuclear reactor as dramatic changes in mechanical properties (i.e. embrittlement) may result in fuel cladding failure and undesired radioactivity release. Thus, the development of mechanical testing techniques on the mesoscale enables one to obtain data from small volumes (e.g. produced by ion irradiation) and samples with larger (bulk) volumes irradiated by neutrons to obtain data that is essential to further validate mechanical testing of ion irradiated alloys and advance materials development for next generation nuclear reactors such as those being developed in DOE's Nuclear Energy Programs.

Publications

Journal Articles

Gigax, J. G., A. J. Torrez, Q. Mcculloch, H. Kim, S. A. Maloy and N. Li. Sizing up mechanical testing: Comparison of microscale and mesoscale mechanical testing techniques on a FeCrAl welded tube. Submitted to *Journal of Materials Research*. (LA-UR-19-32551)

*Gigax, J. G., H. Vo, Q. McCulloch, M. Chancey, Y. Wang, S. A. Maloy, N. Li and P. Hosemann. Micropillar compression response of femtosecond laser-cut single crystal Cu and proton irradiated Cu. 2019. *Scripta Materialia*. **170**: 145-149. (LA-UR-19-21957 DOI: 10.1016/j.scriptamat.2019.05.004)

*Gigax, J. G., J. K. Baldwin, C. J. Sheehan, S. A. Maloy and N. Li. Microscale shear specimens for evaluating the shear deformation in single-crystal and nanocrystalline Cu and at Cu–Si interfaces. 2019. *Journal of Materials Research*. **34** (9): 1574-1583. (LA-UR-19-21222 DOI: 10.1557/jmr.2019.104)

Gigax, J. G., O. El Atwani, Q. Mcculloch, B. Aytuna, M. Efe, S. J. Fensin, S. A. Maloy and N. Li. Micro- and mesoscale mechanical properties of an ultra-fine grained FeCrMnNi high entropy alloy produced by large strain machining. Submitted to *Scripta Materialia*. (LA-UR-19-29789)

Mcculloch, Q., J. G. Gigax and P. Hosemann. Femtosecond laser ablation for mesoscale specimen evaluation. Submitted to *JOM*. (LA-UR-19-27649)

Reports

Gigax, J. G., H. Kim, M. R. Chancey, Y. Wang and N. Li. Heavy Ion Irradiation Characterization of C26M. Unpublished report. (LA-UR-20-28209)

Gigax, J. G. and N. Li. Microstructural and Nanomechanical Characterization of FeCrAl Pressure Resistance Welds. Unpublished report. (LA-UR-20-27950)

Presentation Slides

Gigax, J. G., N. Li, Q. Mcculloch, H. Kim, M. R. Chancey, Y. Wang, C. R. Lear, S. A. Maloy and P. Hosemann. Novel Small Scale Mechanical Testing Techniques for Nuclear Materials. Presented at *TMS 2021 Spring (online)*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21722)

Gigax, J. G., N. Li and S. A. Maloy. Nb Weld Overview. . (LA-UR-20-26513)

Gigax, J. G., O. El Atwani, M. R. Chancey, J. K. S. Baldwin and S. A. Maloy. Nanomechanical Properties of Pristine and Heavy Ion Irradiation Nanocrystalline Tungsten. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-28. (LA-UR-20-21593)

Gigax, J. G., Q. Mcculloch, S. A. Maloy, P. Hosemann and N. Li. Femtosecond laser ablation techniques for mesoscale specimen analysis. Presented at *University of California Berkeley Mechanics Workshop*, Berkeley, California, United States, 2020-03-02 - 2020-03-03. (LA-UR-20-21927)

Gigax, J. G., S. A. Maloy and N. Li. Novel micro- and mesoscale techniques for mechanical property characterization and their applications. . (LA-UR-21-20723)

Posters

Gigax, J. G., N. Li and S. A. Maloy. Micro- and Mesoscale Mechanical Methods for Material Extremes. Presented at *Materials Capability Review 2020*, Los Alamos, New Mexico, United States, 2020-04-30 - 2020-04-30. (LA-UR-20-22896)

Gigax, J. G., O. El Atwani, Q. Mcculloch, B. Aytuna, M. Efe, S. J. Fensin, S. A. Maloy and N. Li. Micro- and mesoscale mechanical properties of an ultra-fine grained CrFeMnNi high entropy alloy produced by large strain machining. Presented at *TMS 202*, San Diego, California, United States, 2020-02-23 - 2020-02-28. (LA-UR-20-21399)

Other

Gigax, J. G., T. Ajantiwalay and S. A. Maloy. Compression of mesoscale pillars in unirradiated HT9 and HT9 irradiated with protons up to 0.1 dpa. Audio/Visual. (LA-UR-20-28091)

Ferromagnetism and Spin Fluctuations in the Atomically-Thin Limit

Scott Crooker
20180747PRD3

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 an entirely new route towards achieving magnetism in a new class of 2D materials based on the semiconductor gallium selenide (GaSe). Recent theory indicates that magnetic behavior can be induced in GaSe by electrical means. Electrically-controllable magnetism is a longstanding 'holy grail' 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

Crooker, S. A., M. Goryca, J. Li, S. Tongay, K. Yumigeta and H. Li. Carrier-density-dependent valley relaxation in a monolayer semiconductor and the role of substrate-induced disorder. Submitted to *Physical Review Applied*. (LA-UR-21-20744)

Crooker, S. A., P. Schiffer, M. M. Goryca, C. Nisoli, J. Li, C. Leighton, X. Zhang, J. Watts and A. Balk. Field-Induced Monopole Plasma in Artifcial Spin Ice. Submitted to *Nature*. (LA-UR-20-24139)

*Goryca, M., J. Li, A. V. Stier, T. Taniguchi, K. Watanabe, E. Courtade, S. Shree, C. Robert, B. Urbaszek, X. Marie and S. A. Crooker. Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields. 2019. *Nature Communications*. **10** (1): 4172. (LA-UR-19-23579 DOI: 10.1038/s41467-019-12180-y)

Li, J., S. A. Crooker, M. M. Goryca, A. V. Stier, N. Wilson and X. Xu. Spontaneous Valley Polarization of Interacting Carriers in a Monolayer Semiconductor. 2020. *Physical Review Letters*. **125** (14): 147602. (LA-UR-20-25746 DOI: 10.1103/PhysRevLett.125.147602)

Posters

Li, J. and J. Zhu. Probing Quantum Hall and Quantum Valley Hall Effect in Bilayer Graphene Nanostructures. Presented at *The 46th Conference on the Physics and Chemistry of Surfaces and Interfaces (PCSI-46)*, Santa Fe, Minnesota, United States, 2019-01-13 - 2019-01-17. (LA-UR-19-20395)

Overcoming the Curse of Dimensionality to Predict Chemical Reactivity

Beth Lindquist
20180758PRD4

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.

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)

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 Applied to Physically Informed Models. Submitted to *Journal of Chemical Physics*. (LA-UR-21-21954)

*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)

Sherman, Z. M., M. P. Howard, B. A. Lindquist, R. B. Jadrich and T. M. Truskett. Inverse methods for design of soft materials. Submitted to *Journal of Chemical Physics*. (LA-UR-20-20466)

Presentation Slides

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)

A Novel “Three-in-One” Metal Organic Framework-Based Platform For Nanoparticle Encapsulation and Organization

Jennifer Hollingsworth
20190620PRD1

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.

Publications

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)

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

Vivien Zapf
20190623PRD2

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.

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)

In Situ Mesoscale Response under Combined Pressure-Shear Dynamic Loading

Darby Luscher
20190639PRD2

Project Description

A combined experiment and theory approach will be developed to perform in situ measurements of materials under pressure-shear shock loading. This work will result in better understanding of the mesoscale material deformation mechanisms and a computational model for simulating the material response. This work directly addresses the national security challenges related to the dynamic behavior of materials. The ability to understand and simulate pressure-shear shock conditions in low symmetry materials will be immediately useful to the mission areas of Dynamic Mesoscale Materials Science and to Stockpile Stewardship.

Publications

Journal Articles

Zuanetti, B., D. J. Luscher, K. J. Ramos, C. A. Bolme and V. Prakash. Dynamic flow stress of pure polycrystalline aluminum: Pressure-shear plate impact experiments and extension of dislocation-based modeling to large strains. 2021. *Journal of the Mechanics and Physics of Solids*. **146**: 104185. (LA-UR-20-23354 DOI: 10.1016/j.jmps.2020.104185)

Posters

Zuanetti, B., C. A. Bolme, K. J. Ramos and D. J. Luscher. Investigation of the Mesoscale Response of Anisotropic Crystals under Combined Pressure-Shear Dynamic Loading. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27842)

Synthesis of Platinum-Rare Earth Intermetallic Fuel Cell Catalysts

Jacob Spendelow
20190640PRD3

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.

Publications

Journal Articles

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., 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)

Ex Machina Hamiltonians for Next-Generation Molecular Simulations

Galen Craven
20190642PRD3

Project Description

The project will apply advanced computer simulation methods to examine the molecular mechanisms underlying electrical and thermal conduction processes in emerging energy nanotechnologies with direct applications to sustainable energy initiatives. The two specific applications to be explored are electronic conduction in molecular nanodevices that operate at the human-machine interface and heat conduction in complex molecular devices. This proposal will advance the current understanding of molecular-level functionality in several energy nanotechnologies and could significantly impact DOE missions related to energy independence.

Publications

Journal Articles

*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)

Presentation Slides

Craven, G. T. Data-Driven Determination of Correlation Functions. . (LA-UR-20-24825)

Other

Craven, G. T. Dataset and programs to calculate properties of a Lennard-Jones fluid. Dataset. (LA-UR-20-24204)

Designing New Ferroelectric Materials with Spin Crossover Transitions

Wanyi Nie
20190647PRD3

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.

Publications

Journal Articles

Owczarek, M. T., P. Szklarz and R. Jakubas. Towards ferroelectricity-inducing chains of halogenoantimonates(III) and halogenobismuthates(III). Submitted to *Angewandte Chemie - International Edition*. (LA-UR-20-28039)

The Optoelectronic Device Applications of 2-Dimensional Interlayer Moiré Excitons

Han Htoon

20190648PRD3

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.

Exploration of Colossal Thermoelectric Power in 4f and 5f Topological Magnets

Filip Ronning
20190654PRD4

Project Description

This research project is well aligned with the Laboratory agenda on quantum information science. Topological materials are widely believed to provide a route to harnessing new functionality in quantum materials in the future. This research is designed to understand the origin of large topological effects in strongly correlated magnetic metals, which are particularly strong in actinide-based materials. The Berry curvature of a wavefunction creates an anomalous velocity, which produces large transverse voltages in topological materials. The large transverse voltage response has potential interest for spintronic applications, as well as developing fundamentally new states of matter. Here we will study how this large response varies as a function of alloying various actinide materials. This research will help elucidate the origin of large responses in materials, and hopefully demonstrate how to control their effects.

Publications

Journal Articles

*Asaba, T., S. M. Thomas, M. Curtis, J. D. Thompson, E. D. Bauer and F. Ronning. Anomalous Hall effect in the kagome ferrimagnet. 2020. *Physical Review B*. **101** (17): 174415. (LA-UR-20-20100 DOI: 10.1103/PhysRevB.101.174415)

Asaba, T., V. Ivanov, S. M. Thomas, S. Savrasov, J. D. Thompson, E. D. Bauer and F. Ronning. Colossal anomalous Nernst effect in a correlated noncentrosymmetric kagome ferromagnet. Submitted to *Science Advances*. (LA-UR-21-22548)

Hamann, D. M., S. P. Rudin, F. Ronning, T. Asaba, D. L. M. Cordova, P. Lu and D. C. Johnson. Emergent Structures and Properties in Interface Stabilized 2D-Layers. Submitted to *Science*. (LA-UR-19-31418)

Presentation Slides

Asaba, T., V. Ivanov, S. M. Thomas, S. Savrasov, J. D. Thompson, E. D. Bauer and F. Ronning. Colossal anomalous Nernst effect in a correlated noncentrosymmetric kagome ferromagnet. Presented at *APS march meeting 2021 (online)*, Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-21064)

Defect tolerant scintillators: Linking structure and performance via machine learning (ML)

Blas Uberuaga

20190656PRD4

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.

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)

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)

Development of Next Generation Microstructure-aware Burn Models for High Explosives.

Tariq Aslam
20190658PRD4

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.

Importance of Metal/Oxide Interfaces to Design and Tailor Composite Material Properties.

Blas Uberuaga
20200676PRD1

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 and National Nuclear Security Administration.

Publications

Journal Articles

Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Interplay between defect transport and cation spin frustration in corundum-structured oxides. Submitted to *Physical Review Letters*. (LA-UR-20-28924)

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)

Banerjee, A., E. F. Holby, A. A. Kohnert and B. P. Uberuaga. Thermodynamics of Vacancy formation in Fe2O3: role of exchange-correlation functionals and system size. Submitted to *Small*. (LA-UR-20-24936)

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)

Strain Susceptibility of Quantum Critical Fluctuations

Ross Mcdonald
20200680PRD1

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

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)

Electrically Pumped Laser Diodes Using Charged Colloidal Quantum Dots

Victor Klimov
20200685PRD2

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

Presentation Slides

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)

Design and Discovery of Novel, Two-Dimensional f-electron Quantum Materials

Eric Bauer
20200686PRD2

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.

Atomistic Modeling and Machine Learning for Bio-advantaged Polymer Design

Ghanshyam Pilania
20200688PRD2

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.

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)

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)

Design and Discovery of Novel High-entropy Alloys

Saryu Fensin
20200755PRD3

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, we 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 us the capability to develop materials with tailored properties that will be indispensable to various projects within the National Nuclear Security Administration.

Publications

Journal Articles

Lee, C., F. Maresca, R. Feng, Y. Chou, T. Ungar, M. Widom, K. An, J. Poplawsky, Y. Chou, P. K. Liaw and W. A. Curtin. Strength Can be Controlled by Edge Dislocations in Refractory High-Entropy Alloys. Submitted to *Nature Communications*. (LA-UR-21-22188)

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., Y. Chou, G. Kim, M. C. Gao, K. An, J. Brechtl, C. Zhang, W. Chen, J. Poplawsky, G. Song, Y. Ren, Y. Chou and P. K. Liaw. Lattice-Distortion-Enhanced Yield Strength in a Refractory High-entropy Alloy. Submitted to *Advanced Materials*. (LA-UR-20-27498)

Presentation Slides

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. 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)

Topological Superconductivity in Van Der Waals Materials as a Platform for Qubits

Jianxin Zhu
20200756PRD3

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.

Publications

Journal Articles

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. Drucker, N. H. Jo, B. Kuthanazhi, Z. Huang, C. A. Lane, S. L. Bud'Ko, J. Zhu, P. C. Canfield and J. E. Hoffman. Spin-polarized imaging of strongly interacting fermions in the ferrimagnetic state of Weyl candidate CeBi. Submitted to *Physical Review Letters*. (LA-UR-20-28429)

Peng, S., C. A. Lane, Y. Hu, M. Guo, X. Chen, M. Matzelle, Z. Sun, M. Hashimoto, D. H. Lu, Z. X. Shen, T. Wu, X. H. Chen, R. S. Markiewicz, Y. Wang, A. Bansil, S. D. Wilson and J. F. He. Electronic nature of the pseudogap in electron-doped Sr2IrO4. Submitted to *Nature Physics*. (LA-UR-20-26487)

Winter, G., M. Matzelle, C. A. Lane and A. Bansil. Fully-Compensated Ferrimagnetic Spin Filter Materials within the CrMNAl Equiatomic Quatnernary Heusler Alloys. Submitted to *Journal of Applied Physics*. (LA-UR-20-28904)

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)

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)

Electrically Driven Optoelectronic Plasmonic Nanodevice in Carbon Nanotubes

Andrew Jones
20200757PRD3

Project Description

Photonic systems lie at the heart of almost all modern technologies. They make high speed internet possible and can be found inside of your computers and television sets. This project aims toward developing a new class of ultra-compact and efficient infrared light emitters by exploiting a novel phenomenon called plasmonic, which involves the coupling between light and electrons with materials. The photonic devices less than 1 nanometer thick can be fabricated by using single nanostructures, called nanotubes, as building blocks for information transmission and light emission. These building blocks can also be integrated into existing silicon (Si) based electronic and photonic integrated circuits.

A Gruneisen Approach to Quantum Criticality

Priscila Rosa
20170667PRD1

Project Description

An important aspect of the Department of Energy (DOE) mission is the discovery and manipulation of new quantum states of matter that could lead to entirely new energy relevant technologies. This project will develop a new capability of thermal expansion measurements under extreme conditions that will enable understanding and control of quantum phase transitions and the quantum states that emerge from them.

Technical Outcomes

This project succeeded in its major goal of developing a new experimental capability using strain gauges under applied pressure to measure the thermal expansion of materials. This capability, combined with other thermodynamic probes, provides a powerful toolkit to investigate phase transitions. A breadth of quantum materials were investigated here, ranging from superconductors to antiferromagnets. This project not only impacts existing Department of Energy (DOE)/ Office of basic Energy Science (BES) programs at Los Alamos, but also has stimulated proposals relevant to the Laboratory's national security mission.

Publications

Journal Articles

*Jung, S., S. Seo, S. Lee, E. D. Bauer, H. Lee and T. Park. A peak in the critical current for quantum critical superconductors. 2018. *Nature Communications*. **9** (1): 434. (LA-UR-18-26340 DOI: 10.1038/s41467-018-02899-5)

Ferrari Silveira Rosa, P., S. M. Thomas, F. F. Balakirev, J. B. Betts, S. Seo, E. D. Bauer, J. D. Thompson and M. Jaime. An FBG Optical Approach to Thermal Expansion Measurements under Hydrostatic Pressure. Submitted to *Sensors*. (LA-UR-18-30370)

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)

*Seo, S., X. Wang, S. M. Thomas, M. C. Rahn, D. Carmo, F. Ronning, E. D. Bauer, R. D. dos Reis, M. Janoschek, J. D. Thompson, R. M. Fernandes and P. F. S. Rosa. Nematic State in CeAuSb2. 2020. *Physical Review X*. **10** (1): 011035. (LA-UR-19-27666 DOI: 10.1103/PhysRevX.10.011035)

Toward Controlled Synthesis of Actinide Oxide Nanocrystals: A Theoretical Perspective

Gaoxue Wang
20170670PRD1

Project Description

The long-term goal of this project is to build the knowledge foundation of structures, energetics, and chemical and physical characteristics of tetravalent actinide nanocrystals as a function of particle size, composition, and surface ligands, using a novel high-performance computational framework. Understanding, predicting, and controlling their formation and chemical reactivity is crucial to improve the efficiency of the nuclear fuel cycle, long-term management of nuclear waste, and assessment of contaminated sites.

Technical Outcomes

This project has built knowledge foundation for the interfacial chemistry of actinide nanocrystals (NCs) and organic surface ligands using first-principles simulation. The team has calculated the ligand-surface interaction and performed NCs morphology prediction using analytical models. The knowledge gained from this project explains the morphologies of actinide dioxide NCs observed in experiments, which are key for the controlled synthesis of NCs with different size and shape for targeted applications.

Publications

Journal Articles

Wang, G., E. R. Batista and P. Yang. Nature of excess electrons on reduced AnO2 (111) surfaces (An = Th, U, Pu): From delocalization to localization. Submitted to *Journal of the American Chemical Society*. (LA-UR-18-29910)

*Wang, G., E. R. Batista and P. Yang. Ligand induced shape transformation of thorium dioxide nanocrystals. *Physical Chemistry Chemical Physics*. **20** (26): 17563-17573. (LA-UR-17-31042 DOI: 10.1039/C8CP00240A)

*Wang, G., P. Yang, N. A. Moody and E. R. Batista. Overcoming the quantum efficiency-lifetime tradeoff of photocathodes by coating with atomically thin two-dimensional nanomaterials. 2018. *npj 2D Materials and Applications*. **2** (1): 17. (LA-UR-17-26824 DOI: 10.1038/s41699-018-0062-6)

Wang, G., P. Yang and E. R. Batista. Computational screening of 2D coatings for semiconducting photocathodes. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-29869)

Valley Dynamics and Coherence in Atomically-Thin Semiconductors

Scott Crooker
20170672PRD2

Project Description

The goal of this project is to study a new class of recently discovered semiconductors that are only a single atomic layer thick. These "two-dimensional" semiconductors hold great promise for future applications in ultra-light-weight and low-power electronics.

Technical Outcomes

Work performed in this project successfully measured the intrinsic electron and hole valley relaxation timescales in monolayer semiconductors, using a novel noise-based spectroscopy, and also used high magnetic fields to reveal fundamental materials parameters such as exciton mass and dielectric constants. The results were published in the high-profile journals Science Advances and also Nature Communications. These parameters are essential ingredients for future generations of 2D optoelectronic and valleytronic devices based on 2D semiconductors.

Publications

Journal Articles

Crooker, S. A., M. Goryca, J. Li, S. Tongay, K. Yumigeta and H. Li. Carrier-density-dependent valley relaxation in a monolayer semiconductor and the role of substrate-induced disorder. Submitted to *Physical Review Applied*. (LA-UR-21-20744)

Crooker, S. A., P. Schiffer, M. M. Goryca, C. Nisoli, J. Li, C. Leighton, X. Zhang, J. Watts and A. Balk. Field-Induced Monopole Plasma in Artifcial Spin Ice. Submitted to *Nature*. (LA-UR-20-24139)

*Goryca, M., J. Li, A. V. Stier, T. Taniguchi, K. Watanabe, E. Courtade, S. Shree, C. Robert, B. Urbaszek, X. Marie and S. A. Crooker. Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields. 2019. *Nature Communications*. **10** (1): 4172. (LA-UR-19-23579 DOI: 10.1038/s41467-019-12180-y)

*Goryca, M., N. P. Wilson, P. Dey, X. Xu and S. A. Crooker. Detection of thermodynamic “valley noise” in monolayer semiconductors: Access to intrinsic valley relaxation time scales. 2019. *Science Advances*. **5** (3). (LA-UR-18-27841 DOI: 10.1126/sciadv.aau4899)

Li, J., S. A. Crooker, M. M. Goryca, A. V. Stier, N. Wilson and X. Xu. Spontaneous Valley Polarization of Interacting Carriers in a Monolayer Semiconductor. 2020. *Physical Review Letters*. **125** (14): 147602. (LA-UR-20-25746 DOI: 10.1103/PhysRevLett.125.147602)

Presentation Slides

Goryca, M. M., A. Lopion, K. Nogajewski, M. Potemski and P. Kossacki. Temperature dependence of photoluminescence lifetimes of WSe2 monolayer. Presented at *APS March Meeting*, Los Angeles, Colorado, United States, 2018-03-04 - 2018-03-04. (LA-UR-18-21719)

Goryca, M. M., T. Kazimierczuk, M. Koperski, T. Smolenski, W. Pacuski, A. Golnik, P. Kossacki, P. Wojnar and G. Karczewski. Single magnetic ion in a quantum dot as a memory device. Presented at *XII Symposium of the Institute of Theoretical Physics, University of Warsaw*, Warsaq, Poland, 2017-12-08 - 2017-12-09. (LA-UR-18-22488)

Posters

Goryca, M. M. Detection of thermodynamic “valley noise” in monolayer semiconductors: access to intrinsic valley relaxation timescales. Presented at *46th Conference on the Physics and Chemistry of Surfaces and Interfaces (PCSI-46)*, Santa Fe, New Mexico, United States, 2019-01-13 - 2019-01-17. (LA-UR-19-20396)

Goryca, M. M., J. Li, A. V. Stier, E. Courtade, S. Shree, C. Robert, B. Urbaszek, X. Marie and S. A. Crooker. Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields.. Presented at *NSF site visit*, Tallahassee, Florida, United States, 2019-09-05 - 2019-09-05. (LA-UR-19-28676)

Engineering Deoxyribonucleic Acid (DNA) Protected Silver Nanoclusters via Doping and Alloying

Peter Goodwin
20170688PRD3

Project Description

Developing stable and bright taggants for commerce, wellness detection and national security is a grand challenge. Nanoclusters are collections of a few atoms of metal, where even one extra atom can drastically change the fluorescent properties. We will develop precisely tuned clusters that have defined fluorescence, as a result of the atom tuning. Once successful, these clusters can be used to better detect biothreat agents and tag commodities important in threat reduction.

Technical Outcomes

This project identified the florescence origin of a dual emissive DNA-templated silver nanoclusters system by fluorescence cross-correlation spectroscopy (FCCS). The team discovered the two distinct and separately emissive silver nanoclusters can be templated by the same DNA sequence under identical synthetic conditions. The team studied the structural transformation of an atomically precise gold nanocluster superlattice under high pressure. The stress induced crystal phase transition of gold naoclusters is of fundamental importance for nanoparticle based assembly of functional materials.

Publications

Journal Articles

*Chen, Y., M. L. Phipps, J. H. Werner, S. Chakraborty and J. S. Martinez. DNA Templated Metal Nanoclusters: From Emergent Properties to Unique Applications. 2018. *Accounts of Chemical Research*. **51** (11): 2756-2763. (LA-UR-18-25907 DOI: 10.1021/acs.accounts.8b00366)

Presentation Slides

Chen, Y. Pathogen lights: Fast-testing for food safety. . (LA-UR-19-23194)

Chen, Y. Pathogen Light: Fluorescent Probe for Rapid Foodborne Bacteria Detection. . (LA-UR-19-23193)

Chen, Y. and J. Martinez. NanoCluster Beacons: A Spotlight on DNA Targets. . (LA-UR-18-23524)

Accelerated Discovery of New Nanocomposites for Energy Applications

Aiping Chen
20170691PRD4

Project Description

Accelerated discovery of promising materials to achieve U.S. DOE's goal of developing advanced water splitting materials with enhanced performance and durability for hydrogen generation.

Technical Outcomes

This project investigated the synthesis of oxide nanocomposites and explored their energy applications. Using the well-defined carbon dots (CDs) arrays loaded zeolitic imidazolate framework-8 anchored on one dimensional (1D) zinc oxide (ZnO) nanocomposites, significantly enhanced photoelectrochemical (PEC) water splitting properties were reported. In addition, this project also explored the synthesis of strontium titanate (SrTiO3, STO): magnesium oxide (MgO) nanocomposites. Via chemical etching, obtained novel STO nanostructures showed enhanced Photoelectrochemical (PEC) properties. Simple extension of such strategies is expected to synthesize different oxide nanocomposites for energy applications.

Publications

Journal Articles

*Han, H., S. Kment, F. Karlicky, L. Wang, A. Naldoni, P. Schmuki and R. Zboril. Sb-Doped SnO2 Nanorods Underlayer Effect to the \xce\xb1-Fe2O3 Nanorods Sheathed with TiO2 for Enhanced Photoelectrochemical Water Splitting. 2018. *Small*. **14** (19): 1703860. (LA-UR-18-21360 DOI: 10.1002/smll.201703860)

Presentation Slides

Han, H. Morphological Control Effect of Hierarchical Heterostructure Fe2O3/TiO2 for Photoelectrochemical Water Splitting. Presented at *ECS conference 2018*, Seattle, Washington, United States, 2018-05-12 - 2018-05-12. (LA-UR-18-24154)

Han, H. The synthesis of one dimensional nanostructure for energy storage application. . (LA-UR-19-25579)

Excited State Dynamics for Photochemistry and Light-Matter Interactions

Yu Zhang
20170695PRD4

Project Description

This project will use and develop nonadiabatic excited state molecular dynamics, a software package acknowledged by NNSA for open source, to provide novel computational capabilities critical for understanding light-induced dynamics in many technologically relevant materials. The developed capabilities will have extremely broad applications relevant to the current and future Los Alamos National Laboratory/DOE missions, particularly benefitting the primary goal of the Materials for the Future focus area and in the future modeling of materials important for Los Alamos National Laboratory core mission, such as explosives. The project will develop a new computational capability that can be applied to advance modeling of photostability and optical initiation in high explosives involving bond breaking pathways. The high level goals of the project are to develop a modeling capability to describe the light-induced bond breaking reactions in realistic materials and to apply the capability for the prediction, control and design of specific material properties. In addition, our advance will set the stage for the future abilities to model spin and charge dynamics in electronic materials, transition-metal complexes, as well as general photocatalysis phenomena.

Technical Outcomes

The project developed a first-ever computational capability for modeling photochemistry and strong light-matter interactions for large systems. The capabilities allow for the direct modeling of photoexcitation induced bond breaking, and photochemistry in the cavity. The results lay the important groundwork for prediction, control, and design of materials' functionalities. The work on plasmon mediated reactions may open a door for simulating plasmon-stimulated photochemical processes and help the optimization and control of these new catalytic instruments.

Publications

Journal Articles

*Jiang, H. and Y. Zhang. Preferred states of open electronic systems. 2019. *Physics Letters A*. **383** (24): 2878-2882. (LA-UR-19-26160 DOI: 10.1016/j.physleta.2019.06.035)

*Lystrom, L., Y. Zhang, S. Tretiak and T. Nelson. Site-Specific Photodecomposition in Conjugated Energetic Materials. 2018. *The Journal of Physical Chemistry A*. **122** (29): 6055-6061. (LA-UR-18-24161 DOI: 10.1021/acs.jpca.8b04381)

Nelson, T. R., A. J. White, J. A. Bjorgaard, A. E. Sifain, Y. Zhang, B. T. Nebgen, S. Fernandez-Alberti, D. V. Mozyrsky, S. Tretiak and A. E. Roitberg. Non-adiabatic Excited State Molecular Dynamics: theory and applications for modeling photophysics in extended molecular materials. Submitted to *Chemical Reviews*. (LA-UR-19-25569)

*Wu, Q., L. Zhou, G. C. Schatz, Y. Zhang and H. Guo. Mechanistic Insights into Photocatalyzed H2 Dissociation on Au Clusters. 2020. *Journal of the American Chemical Society*. **142** (30): 13090-13101. (LA-UR-20-23183 DOI: 10.1021/jacs.0c04491)

*Wu, X., R. Wang, Y. Zhang, B. Song and C. Yam. Controllable Single-Molecule Light Emission by Selective Charge Injection in Scanning Tunneling Microscopy. 2019. *The Journal of Physical Chemistry C*. **123** (25): 15761-15768. (LA-UR-19-25118 DOI: 10.1021/acs.jpcc.9b02198)

*Zhang, Y., T. Nelson, S. Tretiak, H. Guo and G. C. Schatz. Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. 2018. *ACS Nano*. **12** (8): 8415-8422. (LA-UR-18-24121 DOI: 10.1021/acsnano.8b03830)

*Zhang, Y., T. Nelson and S. Tretiak. Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. 2019. *Journal of Chemical Theory and Computation*. **151** (15): 154109. (LA-UR-19-24300 DOI: 10.1063/1.5116550)

*Zhang, Y., T. R. Nelson and S. Tretiak. Nonadiabatic Excited-State Molecular Dynamics for Open-Shell Systems. 2020. *Journal of Chemical Theory and Computation*. **16** (4): 2053-2064. (LA-UR-19-29917 DOI: 10.1021/acs.jctc.9b00928)

Conference Papers

Zhang, Y. Plasmonic Hot-Carrier-Mediated Solar Energy Conversion and Tunable Photochemical Reactions.

Presented at *The 10th International Conference on Metamaterials, Photonic Crystals and Plasmonics*. (Lisbon, Portugal, 2019-07-22 - 2019-07-26). (LA-UR-19-20076)

Zhang, Y., T. R. Nelson, S. Tretiak, H. Guo, C. Yam and G. C. Schatz. Plasmonic Hot-Carrier-Mediated Solar Energy Conversion and Tunable Photochemical Reactions. Presented at *The 10th International Conference on Metamaterials, Photonic Crystals and Plasmonics*. (Lisbon, Portugal, 2019-07-22 - 2019-07-26). (LA-UR-19-21628)

Books/Chapters

Zhang, Y., T. R. Nelson and S. Tretiak. Atomistic Simulations of Plasmon Mediated Photochemistry. (LA-UR-19-22815)

Reports

Nelson, T. R. Excited State Dynamics for Photochemistry and Light-Matter Interactions. Unpublished report. (LA-UR-18-25439)

Zhang, Y. Non-adiabatic Excited State Molecular Dynamics Modeling of Photochemistry and Polariton Chemistry. Unpublished report. (LA-UR-21-20629)

Zhang, Y. and T. R. Nelson. Non-adiabatic Excited State Molecular Dynamics Modeling of Photochemistry and Polariton Chemistry. Unpublished report. (LA-UR-19-28554)

Presentation Slides

Zhang, Y. Non-Adiabatic Molecular Dynamics for Strong Light-Matter Interaction. Presented at *257th ACS National Meeting, Orlando 2019*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22862)

Zhang, Y. Plasmonic Hot-Carriers for Solar Energy Conversion & Photochemical Reactions. Presented at *META 2019, the 10th International Conference on Metamaterials, Photonic Crystals and Plasmonics*, Lisbon, Portugal, 2019-07-23 - 2019-07-23. (LA-UR-19-26864)

Zhang, Y. Theory and Modeling of Non-Equilibrium Electron Transport and Energy Conversion. . (LA-UR-19-25320)

Zhang, Y. Atomistic Understanding of Plasmon Mediated Photochemical Reactions\xc2\xa0. Presented at *Virtual International Seminar on Theoretical Advancements*, los alamos, New Mexico, United States, 2020-12-17 - 2020-12-17. (LA-UR-20-30317)

Zhang, Y. Non-adiabatic Excited State Molecular Dynamics Modeling of Photochemistry and Polariton Chemistry. . (LA-UR-21-20630)

Atomic Layer Deposition of Templated Electrode Structures for Electrochemical Devices

Jacob Spendelow
20180711PRD2

Project Description

Energy security, including the limited availability of domestic energy resources and the need to replace fossil fuels with clean energy alternatives, is a major national challenge. Electrochemical energy storage and conversion technologies, including batteries and fuel cells, could enable a faster transition to clean energy sources such as solar and wind, and could help reduce our national dependence on imported petroleum for transportation. Current batteries and fuel cells are limited by unsatisfactory electrode performance, causing decreased efficiency, slow charging, and poor lifetime. The proposed project will yield new electrode structures with enhanced performance and durability, enabling batteries and fuel cells to have higher power, increased robustness, and longer lifetimes. By accelerating the deployment of batteries and fuel cells, the project will enable a more rapid transition to a new clean energy economy.

Technical Outcomes

High temperature polymer electrolyte membrane fuel cells that operate above 100 Celsius without humidification offer advantages in enhanced catalytic activity and carbon monoxide tolerance. However, lack of ionomeric electrode binder for controlled, balanced proton conductivity and hydrophobicity have limited the performance of such membrane electrode assemblies. Through development of novel ion conducting electrode materials, high temperature polymer electrolyte membrane fuel cell power performance was doubled compared to current commercially available materials.

Publications

Journal Articles

Kim, Y. S., A. S. Lee, V. Atanasov, E. J. Park, S. Maurya, E. Baca, C. Fujimoto, M. R. Hibbs and J. Kerres. Synergistically integrated phosphonated poly(pentafluorostyrene)s for fuel cells. Submitted to *Nature Materials*. (LA-UR-20-22783)

*Langlois, D. A., A. S. Lee, N. Macauley, S. Maurya, M. E. Hawley, S. D. Yim and Y. S. Kim. A rejuvenation process to enhance the durability of low Pt loaded polymer electrolyte membrane fuel cells. 2018. *Journal of Power Sources*. **396**: 345-354. (LA-UR-17-30764 DOI: 10.1016/j.jpowsour.2018.06.013)

*Lee, A. S., Y. Choe, I. Matanovic and Y. S. Kim. The energetics of phosphoric acid interactions reveals a new acid loss mechanism. 2019. *Journal of Materials Chemistry A*. **7** (16): 9867-9876. (LA-UR-18-31799 DOI: 10.1039/C9TA01756A)

*Maurya, S., A. S. Lee, D. Li, E. J. Park, D. P. Leonard, S. Noh, C. Bae and Y. S. Kim. On the origin of permanent performance loss of anion exchange membrane fuel cells: Electrochemical oxidation of phenyl group. 2019. *Journal of Power Sources*. **436**: 226866. (LA-UR-19-23575 DOI: 10.1016/j.jpowsour.2019.226866)

*Park, E. J., S. Maurya, A. S. Lee, D. P. Leonard, D. Li, J. Y. Jeon, C. Bae and Y. S. Kim. How does a small structural change of anode ionomer make a big difference in alkaline membrane fuel cell performance?. 2020. *Journal of Materials Chemistry A*. **7** (43): 25040-25046. (LA-UR-20-21325 DOI: 10.1039/C9TA10157H)

Posters

S. Lee, A. S., E. J. Park, S. Maurya, V. Atanasov, J. Kerres, H. Jia and Y. S. Kim. Towards Optimization of High Temperature PEMFC Performance with Phosphonated Ionomer Electrodes and Ion-Pair Coordinated Electrolytes. Presented at *Gordon Conference*, Providence, Rhode Island, United States, 2018-07-29 - 2018-08-03. (LA-UR-18-26900)

Doped Carbon Dots for Enhanced Fuel Cell Catalysis

Piotr Zelenay
20180754PRD4

Project Description

This project will use sonochemistry to develop carbon dots-based fuel cell catalysts. The work will focus on dual metallic/nonmetallic-doping as a way of imparting enhanced oxygen reduction reaction activity in carbon dots. This approach is directly aligned with the Laboratory's mission and goals in the area of energy security, and has potential for the development of a new research program at Los Alamos National Laboratory.

Technical Outcomes

Initially, project focused in the use of sonochemistry in the synthesis of oxygen reduction electrocatalysts. Once the approach proved unsuccessful, Dr. Vijay Kumar started a new research topic on the durability of non-precious oxygen reduction catalysts obtaining some promising results. However, in March 2020 he resigned his position and left Los Alamos for reasons unrelated to his research, before completing experiments. The electrocatalyst durability research will be likely continued by another researcher in the future.

Publications

Journal Articles

Kumar, V. B. AS101-Loaded PLGA–PEG Nanoparticles for Autoimmune Regulation and Chemosensitization. 2019. *ACS Applied Bio Materials*. **2** (5): 2246-2251. (LA-UR-19-23090 DOI: 10.1021/acsabm.9b00200)

Books/Chapters

Kumar, V. B. Synthesis of Micro and Nanoparticles of Lignin. (LA-UR-19-23396)

Perovskite-type Metal-Organic Framework with Strong Magnetoelectric Coupling

Hsinhan Tsai
20190613PRD1

Project Description

The project ties closely with Laboratory mission-relevant projects to address challenges in national energy security. The obtained material can be potentially used in low energy consuming devices for information processing. The magnetic based materials offer unique physical properties where the magnetic-electric and optical properties are coupled together, which allows full control over these properties. The full control of these properties is acheived through external triggering, which offers possibility for greatly enhancing the information security.

Technical Outcomes

This project targeted the development of new metal organic material with coupled electrical and magnetic properties. The primary researcher designed and synthesized a series of metal organic materials with manganese-chloride octahedron cages separated by organics. Various organics were chosen to alter the crystal structures to achieve different magnetic and electrical orderings in the system. As a result, this project has achieved 2-dimensional and zero-dimensional magnets by tuning the organics in the structure.

Publications

Journal Articles

Chang, C., H. Huang, H. Tsai, S. Lin, P. Liu, F. Hsu, W. Nie, Y. Chen and L. Wang. Facile fabrication of self-assembly functionalized polythiophene hole transporting layer for high performance perovskite solar cells. Submitted to *Advanced Materials*. (LA-UR-20-24370)

Huang, H., H. Tsai, R. Raja, S. Lin, D. Ghosh, C. Hou, J. Shyue, C. Chang, S. Tretiak, W. Chen, W. Nie, K. Lin and L. Wang. Robust un-encapsulated perovskite solar cells protected by fluorinated fullerene electron transporting layer. Submitted to *Nature*. (LA-UR-20-23214)

Huang, H., Q. Liu, H. Tsai, S. Shrestha, l. Su, P. Chen, Y. Chen, H. Lu, C. Chuang, K. Lin, S. Rwei, W. Nie and L. Wang. A simple one-step method with wide processing window for high quality perovskite mini-module fabrication. Submitted to *Advanced Energy Materials*. (LA-UR-20-27549)

Kinigstein, E. D., H. Tsai, W. Nie, J. C. Blancon, K. G. Yager, K. Appavoo, J. Even, M. G. Kanatzidis, A. D. Mohite and M. Y. Sfeir. Edge States Drive Exciton Dissociation in Hot Cast Ruddlesden-Popper Lead Halide Perovskite Thin Films. Submitted to *ACS Nano*. (LA-UR-20-21239)

*Liu, C., H. Tsai, W. Nie, D. J. Gosztola and X. Zhang. Direct Spectroscopic Observation of the Hole Polaron in Lead Halide Perovskites. 2020. *The Journal of Physical Chemistry Letters*. **11** (15): 6256-6261. (LA-UR-20-24148 DOI: 10.1021/acs.jpclett.0c01708)

*Liu, F., M. Yoho, H. Tsai, K. Fernando, J. Tisdale, S. Shrestha, J. K. Baldwin, A. D. Mohite, S. Tretiak, D. T. Vo and W. Nie. The working principle of hybrid perovskite gamma-ray photon counter. 2020. *Materials Today*. **37**: 27-34. (LA-UR-19-25920 DOI: 10.1016/j.mattod.2020.02.022)

*Tsai, H., C. Liu, E. Kinigstein, M. Li, S. Tretiak, M. Cotlet, X. Ma, X. Zhang and W. Nie. Critical Role of Organic Spacers for Bright 2D Layered Perovskites Light-Emitting Diodes. 2020. *Advanced Science*. **7** (7): 1903202. (LA-UR-19-20440 DOI: 10.1002/advs.201903202)

*Tsai, H., C. Liu, E. Kinigstein, M. Li, S. Tretiak, M. Cotlet, X. Ma, X. Zhang and W. Nie. Critical Role of Organic Spacers for Bright 2D Layered Perovskites Light-Emitting Diodes. 2020. *Advanced Science*. **7** (7): 1903202. (LA-UR-19-25919 DOI: 10.1002/advs.201903202)

*Tsai, H., F. Liu, K. Fernando, B. L. Scott, S. Tretiak, D. T. Vo, J. Strzalka and W. Nie. A sensitive and robust thin-film x-ray detector using 2D layered perovskite diodes. 2020. *Nature*. **6** (15): eaay0815. (LA-UR-19-22971 DOI: 10.1126/sciadv.aay0815)

Tsai, H., W. Huang, R. Vil\xc3\xa1, C. Liu, X. Wen, m. Li, G. Wiederrecht, M. Cotlet, Y. Cui, Z. Zhang, X. Ma and W. Nie. Perovskite Nanocrystals Stabilized in Metal-Organic Frameworks for Bright Light Emitting Diodes. Submitted to *Nature Nanotechnology*. (LA-UR-20-23017)

Zhang, J., H. Tsai, W. Nie and B. Hu. Enabling AC electroluminescence in quasi-2D perovskites by uniformly arranging different-n-value nanoplates to allow bidirectional charge transport. 2020. *Nano Energy*. 105413. (LA-UR-20-25291 DOI: 10.1016/j.nanoen.2020.105413)

Zhou, Y., K. Fernando, J. Wan, F. Liu, S. Shrestha, J. T. Tisdale, H. Tsai, S. Tretiak, H. Huang and W. Nie. Millimeter-size all-inorganic perovskite crystalline thin film grown by chemical vapor deposition. Submitted to *Advanced Functional Materials*. (LA-UR-21-20964)

Posters

Tsai, H., F. Liu, S. Shrestha, K. Fernando, S. Tretiak, B. L. Scott, D. T. Vo, J. Strzalka and W. Nie. Highly Sensitive, Self-powered Thin Film X-ray Detector Using Ruddlesden-Popper Phase Layered Perovskite Diodes. Presented at *LANL Post-Doc Research Day*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28484)

Modernizing Detonator Production and Inspection: Robotics meets Additive and Digital Manufacturing

Alexandria Marchi
20200437MFR

Project Description

This project aims to create a new paradigm for detonator design and manufacturing towards enhancing the technological readiness of our detonator production agency. The Laboratory has the mission to supply detonators to a wide range of explosive operations and missions both at Los Alamos and across the Nuclear Security Enterprise, ranging from research and development tests, to Hydros and proton radiography (pRAD) shots at Los Alamos, to SubCritical Shots at Nevada National Security Site (NNSS) and across the Complex. Through advanced manufacturing investments targeting detonator production, advanced detonator design concepts may be considered, designed, manufactured, and tested all at Los Alamos in a fraction of the time and expense currently required because of extended manufacturing capabilities between industry and multiple complexes. Advanced manufacturing processes are critical for efficient, flexible, and agile responsiveness across the nuclear weapons complex.

Integrating Additive Manufacturing and Investment Casting for Complex Metal Architectures with Predictable Mechanics

Matthew Lee
20200450MFR

Project Description

3-Dimensional (3-D) printed metals can potentially advance several key Department of Energy (DOE)/ National Nuclear Security Administration (NNSA) missions related to stockpile modernization and retrofit, enhanced surveillance, and space applications. However, the properties of printed metals can be difficult to predict and reproduce, and historically this has impeded the adaptation of 3-D printing technology in many applications pertinent to the DOE. This project aims to bridge the gap between old and new technologies by hybridizing 3-D printing with traditional investment casting. The goal is to create new manufacturing techniques wherein 3-D printing is used to create hollow ceramic molds into which metals can be directly cast; this will achieve both the free-form design of printed objects with the predictable and reliable properties of cast metals. We expect to develop a simple collection of manufacturing techniques that can be used to create any castable metal with nearly any 3-D geometry. In turn, this will open up new applications in nuclear weapon design, satellites and other aerospace technologies, and national security, wherein high-precision metal components with exotic design are currently needed to enhance the performance of engineered systems.

Special Carbide for Weapon Applications

David Jablonski
20200461MFR

Project Description

The novel use of a ceramic in weapons has become of increasing interest to the weapons community. This application of the ceramic has very attractive characteristics for use in the nuclear stockpile. The material is challenging to fabricate, but in recent years Los Alamos has made significant advances in the necessary technologies. The objective of this project is to integrate these technologies and demonstrate the fabrication of the material in a form that could be used in a weapon.

Publications

Reports

C. Triola, C. L., C. C. Joggerst, C. Chen, T. J. Foley and D. F. Jablonski. Simulations of Sweeping Wave Propagation in a Boron Carbide Plate. Unpublished report. (LA-UR-20-29040)

The Use of Additive Manufacturing of High Explosives and its Application to Weapon Safety

Von Whitley

20200463MFR

Project Description

This project will investigate the possibility of using additive manufacturing (AM) of high explosives (HE) to produce a structured explosive whose detonation property can be turned on or off depending on the system configuration. In a single component configuration, the structure of the explosive will prevent detonation propagation under any external impulse (unintentional or accidental use). With the addition of a secondary liquid component, the binary mixture will allow a detonation to occur. The secondary component can be either reactive (liquid explosive) or inert (water) depending on performance and safety needs of the application.

Publications

Presentation Slides

J. Coffelt, C. A. Los Alamos Summer Project 2020. . (LA-UR-20-27795)

Mueller, A. H., A. M. Schmalzer, V. H. Whitley, P. R. Bowden and B. C. Tappan. Applications of HE additive manufacturing at LANL. Presented at *JOWOG AM 2020*, livermore, California, United States, 2020-01-27 - 2020-01-30. (LA-CP-20-20039)

Prompt, Photogated Negative Hydrogen Source

Rodney Mccrady
20200468MFR

Project Description

Los Alamos Neutron Science Center (LANSCE) is a particle accelerator at Los Alamos that is used for a variety of basic science and mission-driven experiments. These measurements require a negative hydrogen (H-) ion beam. The current source for this beam uses a plasma as well as a large amount of highly reactive cesium. This makes it very difficult to operate and understand, and often results in reduced performance or even reduced user time as a result. This project will use light, atomic hydrogen, and solid state materials similar to those used in solar cells and sensors to produce the first demonstration of a light controlled H- beam. The individual components required are all heavily used by various industries, largely computing related. This means that the technology for the individual components is extremely well developed. This will make it easier to make a well understood, adaptable source. This experiment will be the first ever demonstration and will give insights on how to scale and optimize the process for a future prototype that could be tested at Los Alamos and could potentially replace the currently used source if successful.

Publications

Journal Articles

Alexander, A. M., M. Gaowei, S. Mistry, J. Walsh, F. Liu, K. Evans-Lutterdot, E. Stavitski, V. Pavlenko, K. Attenkofer, J. M. Smedley and N. A. Moody. Robust method for broadband efficiency enhancement of electron photocathodes using optical interferences. Submitted to *Applied Physics Letters*. (LA-UR-21-22492)

Understanding Homogenization Kinetics of As-Cast Plutonium Alloys to Improve Manufacturing of Weapons Components

Jeremy Mitchell
20200474MFR

Project Description

One of the most time-consuming steps of plutonium (Pu) manufacturing is the post-casting thermal treatment needed to homogenize and stabilize as-cast Pu-Ga (Plutonium-Gallium) alloys. Through careful experiments on a series of well-characterized samples, we will replicate manufacturing processes with in-situ diagnostics to assess the optimal heat treatment for these alloys. This science-based approach to weapons manufacturing will be useful in optimizing the homogenization process and has the potential for time reduction in one step of the plutonium manufacturing process.

Rust, Dust, and a Passive Future - Resilient Actinide Materials

Samantha Lawrence

20200481MFR

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.

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)

In-Situ Ultrasound Grain Refinement in Electron Beam Additive Manufacturing for Improvement of High Strain-Rate Properties

Cristian Pantea
20200500MFR

Project Description

Electron Beam Additive Manufacturing (EBAM) has potential applications with respect to the stewardship of the nation's nuclear weapons stockpile. The resulting metal structure of the EBAM process presents a challenge to the implementation of this technology. Ultrasound excitation applied during the EBAM process could improve the metal structure of the builds, thus making the components intrinsically better. The goal of this research is to determine if coupling an ultrasound source to the component during EBAM fabrication improves the subsequent metal structure. Successful outcome of this research could provide tangible improvements to this developing technology, by improving the resulting mechanical properties of the fabricated components. Many industries would benefit from the result. This project leverages existing technical competencies within Los Alamos and will ensure that the Laboratory remains a leader in the field of EBAM technology.

A Simplified Design and Advanced Manufacture for Expedited Explosive Hydrodynamic Testing and Equation of State Development using Extreme Scaling

Von Whitley
20190530MFR

Project Description

Development of a scaled hydrodynamic test, made with advanced manufacturing, to characterize explosive driven performance for the nuclear explosive package (NEP) is proposed. The proposed methods will assess scaling relationships and produce high quality, high precision parts requiring no explosive machining and will significantly decrease production and qualification time and costs. This has the potential to revolutionize metal/ explosive (or any multi-material explosive assembly) component manufacture and hydrodynamic design and qualification of NEP.

Technical Outcomes

This project produced a design that meets all criteria – simple and fast to manufacture while giving data similar to larger and more complex experiments. This platform can obtain hydrodynamic data on questions thought to be too expensive to answer before. The rapid manufacture of parts has successfully produced metal parts through a combination of metal stamping and back machining. The insert injection molding of the high explosive (HE) continues development with follow-on funding.

Publications

Presentation Slides

Ramos, K. J. and K. A. Berchtold. Brainstorming meeting with Engel, . (LA-CP-20-20122)

Solvent Anode Development for Electrorefining (ER) and Electromagnetic Isotope Separation (EMIS)

Christopher Leibman
20200488MFR

Project Description

This work will advance nuclear weapons production by making plutonium manufacturing processes more efficient and minimize the generation of radioactive wastes compared to existing processing methods. Development of this chemistry will also impact research supporting other Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions related to non-proliferation treaty compliance, nuclear forensics, astrophysics, nuclear weapons science, and medical radioisotope production.

Technical Outcomes

The project team developed a novel chemical processing method applicable to the purification of plutonium as well as recovery of isotopes purified using electromagnetic isotope separation techniques. Solvent anode electro-refining (SAER) was modeled using thermodynamic modeling method to predict the phase behavior of ternary metal solvents and compared to experimental results. Mechanical designs for the collection of high purity isotopes using gallium as a solvent collector were completed and tested using Indium.

Novel in situ Probes of Mesoscale Materials Dynamics

Dmitry Yarotski
20190643DI

Project Description

Understanding materials behavior at the mesoscale is central to designing and realizing new material functionality. Recent advances in X-ray light sources are enabling significant increases in photon flux and coherency that are poised to provide novel insights into the microscopic origins of materials behavior with unprecedented temporal and spatial resolution, high element specificity and sensitivity to buried interfaces. The overarching goal of this project is to apply novel time-resolved in-situ X-Ray techniques to track materials properties under extreme environments of pressure, temperature and magnetic field. Our research efforts are organized in four crosscutting thrusts aimed at: (i) understanding and manipulating ultrafast magnetic dynamics induced by coherent infrared pulses; (ii) ultra-high-speed monitoring of microstructure and property evolution during additive manufacturing process; (iii) probing materials transformations at high pressures, temperatures and strain rates enabled by unique design of pressure cells; and (iv) developing automated real-time data analysis tools for steering the experiments at novel high-repetition rates light sources. We strongly believe that by pursuing these thrusts simultaneously, we will address the most compelling questions in current materials science using the most advanced techniques available to research community, and provide the Laboratory with a vital capability for probing broad range of mission-relevant materials.

Publications

Journal Articles

Biwer, C. M., D. R. Finstad, S. C. Vogel, J. Zhang, M. McKerns, N. S. Johnson and J. P. Ahrens. Spotlight: Automation of Rietveld Analyses Using an Ensemble of Local Optimizations on Distributed-Computing Networks. Submitted to *Journal of Applied Crystallography*. (LA-UR-20-27665)

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)

*Enriquez, E., G. Wang, Y. Sharma, I. Sarpkaya, Q. Wang, D. Chen, N. Winner, X. Guo, J. Dunwoody, J. White, A. Nelson, H. Xu, P. Dowden, E. Batista, H. Htoon, P. Yang, Q. Jia and A. Chen. Structural and Optical Properties of Phase-Pure UO , \xce\xb1-U O , and \xce\xb1-UO Epitaxial Thin Films Grown by Pulsed Laser Deposition. 2020. *ACS Applied Materials & Interfaces*. **12** (31): 35232-35241. (LA-UR-20-24149 DOI: 10.1021/acsami.0c08635)

*Farmer, T. O., E. Guo, R. D. Desautels, L. DeBeer-Schmitt, A. Chen, Z. Wang, Q. Jia, J. A. Borchers, D. A. Gilbert, B. Holladay, S. K. Sinha and M. R. Fitzsimmons. Nanoscale magnetization inhomogeneity within single phase nanopillars. 2019. *Physical Review Materials*. **3** (8): 081401. (LA-UR-19-29646 DOI: 10.1103/PhysRevMaterials.3.081401)

*Li, P., S. Maddali, A. Pateras, I. Calvo-Almazan, S. O. Hruszkewycz, W. Cha, V. Chamard and M. Allain. General approaches for shear-correcting coordinate transformations in Bragg coherent diffraction imaging. Part II. 2020. *Journal of Applied Crystallography*. **53** (2): 404-418. (LA-UR-20-21519 DOI: 10.1107/S1600576720001375)

Li, W., B. Zhu, Q. He, A. Y. Borisevich, C. Yun, R. Wu, P. Lu, Z. Qi, Q. Wang, A. Chen, h. wang, S. A. Cavill, K. H. Zhang and J. MacManus-Driscoll. Interface Engineered Room-Temperature Ferromagnetic Insulating State in Ultrathin Manganite Films. Submitted to *Advanced Sciences*. (LA-UR-20-24152)

Li, W., B. Zhu, R. Zhu, Q. Wang, P. Lu, Y. Sun, C. Cafolla, Z. Qi, A. Chen, P. Gao, H. Wang, Q. He, K. Zhang and J. L. MacManus-Driscoll. Atomic-Scale Control of Electronic Structure and Ferromagnetic Insulating State in Perovskite Oxide Superlattices by Long-Range Tuning of BO Octahedra. 2020. *Advanced Functional Materials*. **30** (40): 2001984. (LA-UR-20-28256 DOI: 10.1002/adfm.202001984)

Pateras, A., R. Harder, W. Cha, J. G. Gigax, J. K. S. Baldwin, J. Tischler, R. Xu, W. Liu, M. Erdmann, R. Kalt, R. Sandberg, S. J. Fensin and R. Pokharel. Combining Laue diffraction with Bragg coherent diffraction imaging at 34-ID-C. Submitted to *Journal of Synchrotron Radiation*. (LA-UR-20-21980)

Pateras, A., R. Harder, W. Cha, J. G. Gigax, J. K. S. Baldwin, J. Tischler, R. Xu, W. Liu, M. Erdmannn, R. Kalt, R. L. Sandberg, S. J. Fensin and R. Pokharel. Combining Laue diffraction with Bragg coherent diffraction imaging at 34-ID-C. Submitted to *Journal of Synchrotron Radiation*. (LA-UR-20-25553)

*Paudel, B., I. Vasiliev, M. Hammouri, D. Karpov, A. Chen, V. Lauter and E. Fohtung. Strain charge mediated magnetoelectric coupling across the magnetic oxide/ferroelectric interfaces. 2019. *RSC Advances*. **9** (23): 13033-13041. (LA-UR-19-29648 DOI: 10.1039/C9RA01503E)

Paudel, B., K. T. Kang, Y. Sharma, H. Nakotte, D. A. Yarotski and A. Chen. Symmetry mismatch controlled ferroelastic domains ordering and functional properties of manganite films on cubic miscut substrates. Submitted to *Nanoscale*. (LA-UR-21-22621)

Sweeney, C. M., C. M. Biwer, A. Quan, B. Sturtevant and L. Q. Huston. Real-time Tools for Analysis of Dynamic Diamond Anvil Cell Experiment Data. Submitted to *Review of Scientific Instruments*. (LA-UR-20-27493)

Reports

Sweeney, C. M., B. Sturtevant, C. M. Biwer, C. A. Bolme, R. C. Huber, L. Q. Huston, E. McBride, L. Miyagi, C. Prescher, K. J. Ramos, J. Smith and T. Turton. Data Science and Computation for Rapid and Dynamic Compression Experiment Workflows at Experimental Facilities Workshop Report. Unpublished report. (LA-UR-20-27469)

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)

Chen, A. Interplay of Strain, Defects and Interface on Functional Properties in Vertical Nanocomposites. Presented at *19th International Conference on Crystal Growth and Epitaxy (ICCGE-19)*, Keystone, Colorado, United States, 2019-07-28 - 2019-08-02. (LA-UR-19-27280)

Chen, A. Correlation among strain, defect, interface and functional properties in oxide nanocomposites. Presented at *CINT user meeting*, los alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27407)

Chen, J., N. E. Hahn and S. J. Fensin. Understanding the Role of Grain Boundary in Inducing Damage and Failure under Dynamic Loading in BCC Ta. Presented at *TMS 2020 Annual Meeting & Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21564)

Choi, Y. J. Applying Neural Networks to Experimental Diffraction Data. . (LA-UR-20-26201)

Huston, L. Q., E. K. Moss, J. S. Smith, R. Husband, Z. Jenei, H. P. Liermann, B. Sturtevant and E. F. O'bannon. Compression rate dependence of the \xce\xb1 to \xcf\x89 phase transition in titanium. Presented at *ACA meeting 2020*, Virtual, New Mexico, United States, 2020-08-02 - 2020-08-02. (LA-UR-20-25893)

Huston, L. Q., E. K. Moss and B. Sturtevant. Dynamic Compression of Ti. . (LA-UR-20-23802)

Huston, L. Q., L. Miyagi, H. P. Liermann, R. Husband and B. Sturtevant. Radial diffraction in the dynamic DAC. Presented at *EuXFEL User Meeting*, Hamburg, Germany, 2020-01-29 - 2020-01-29. (LA-UR-20-20704)

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)

Sturtevant, B. Proposal 2592: dDAC @ EuXFEL: "Ti Team" Kickoff Meeting. Presented at *Proposal 2592 Community Proposal Planning Meeting*, online, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20257)

Sturtevant, B., J. S. Pigott, L. Q. Huston, C. A. Bolme, D. M. Dattelbaum and H. Collaboration. Thermally-induced, quenchable bcc Zr using the European XFEL. Presented at *2020 European XFEL Users' Meeting*, Hamburg, Germany, 2020-01-27 - 2020-01-31. (LA-UR-20-20717)

Sweeney, C. M. Thrust IV: New Automated Real-Time Data Analysis and Data Management Tools. . (LA-UR-20-24282)

Sweeney, C. M., A. Therrien and R. Coffee. Outbrief on LCLS Workshop on Automated Analysis and Control for X-ray Science. Presented at *High Power Laser Workshop*, Menlo Park, California, United States, 2019-09-26 - 2019-09-27. (LA-UR-19-30288)

Sweeney, C. M., C. M. Biwer and A. Quan. Tools and Workflow for Analysis of Dynamic Diamond Anvil Cell Experiment Data. Presented at *EuXFEL/DESY Users Meeting*, Hamburg, Germany, 2020-01-27 - 2020-01-31. (LA-UR-20-20709)

Posters

Huston, L. Q., L. Miyagi, H. P. Liermann, R. Husband and B. Sturtevant. Radial diffraction in the dynamic diamond anvil at ECB. Presented at *EuXFEL User Meeting*, Hamburg, Germany, 2020-01-29 - 2020-01-29. (LA-UR-20-20614)

Pateras, A., R. Harder, W. Cha, J. G. Gigax, J. K. S. Baldwin, J. Tischler, R. Xu, W. Liu, M. Erdmann, R. Kalt, R. L. Sandberg, S. J. Fensin and R. Pokharel. Novel X-ray Tools to Study Size Effects on Nanocrystalline Materials. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21520)

Other

Sturtevant, B., L. Q. Huston, A. Quan, C. M. Biwer and C. M. Sweeney. Data from Dynamic Diamond Anvil Cell Experiment October 2019. Dataset. (LA-UR-20-24551)

Design for Manufacture Pit Feasibility Study

Christina Scovel
20200665DI

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.

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)

Expedited High Explosive Formulation Through Processing-structure-property-performance Relationships

Kyle Ramos
20200667DI

Project Description

After years of stockpile stewardship, we are in a period of “rapidly changing geopolitics wherein inter-state competition, not terrorism, is now the primary concern in United States national security [excerpt from Summary of the 2018 National Defense Strategy of the United States of America, Sharpening the American Military’s Competitive Edge]." Laboratory scientists are being called upon to increase stockpile responsiveness. Our recent achievements in novel processing and pressing methods, using in situ diagnostics and sensors, and direct numerical simulation of plastic bonded explosives (PBXs) at the mesoscale, are reaching a state of maturity sufficient to greatly expedite formulation of high performance, reduced sensitivity PBX, with grain structures optimized for improving safety, mechanical properties, and manufacturability. With this materials science and engineering approach, the United States Nuclear Weapons complex can retain the performance and test history of high melting explosive (HMX)-based formulations such as PBX 9501 while still greatly improving them for use in the current and future stockpile.

Publications

Journal Articles

Powell, M. S., D. S. Moore and S. D. Mcgrane. Insight into The Chemistry of TNT During Shock Compression Through Ultrafast Absorption Spectroscopies. Submitted to *Journal of Chemical Physics*. (LA-UR-20-29986)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Simulating Knoop hardness anisotropy of Al and \xce \xb2-HMX with a crystal plasticity finite element model. Submitted to *International Journal of Plasticity*. (LA-UR-20-28670)

Reports

Powell, M. S., D. S. Moore and S. D. Mcgrane. Response to reviewers- Insight into The Chemistry of TNT During Shock Compression Through Ultrafast Absorption Spectroscopies. Unpublished report. (LA-UR-20-29987)

Saavedra, R. A., J. A. Matteson, K. A. Berchtold and K. J. Ramos. Design of a Slit Rheometer for Characterization of Explosive Formulations. Unpublished report. (LA-CP-20-20665)

Presentation Slides

Powell, M. S., S. D. Mcgrane, R. T. Perriot, C. A. Bolme, D. S. Moore, M. J. Cawkwell and K. J. Ramos. Validating Thermomechanical Models with Stokes, anti-Stokes, Raman Thermometry and Impulsively Stimulated Light Scattering: Experimentally solving the heat equation. . (LA-UR-21-20024)

Powell, M. S., S. D. Mcgrane, R. T. Perriot, C. A. Bolme, D. S. Moore, M. J. Cawkwell and K. J. Ramos. Validating thermomechanical models of cyclotetramethylene tetranitramine (HMX) through impulsively stimulated thermal scattering. Presented at *March APS Meeting -- Virtual*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22177)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Single crystal model for high rate deformation of \xc3\x9f-HMX. Presented at *APS March Meeting 2021*, College Park, Maryland, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22333)

Investigation of the Role of Actinides on the Local Structure of Molten Salts Using Neutron Pair-distribution Function Analysis

Sven Vogel
20200747DI

Project Description

Molten salts play important roles in nuclear processes from actinides processing (including spent fuel processing) to cooling or fuel media for novel reactor concepts (including small modular reactors). Properties of the melts are of paramount importance to understand, control, and optimize these processes and design for these applications. Due to the temperatures involved as well as chemical and radiological hazards involved, typical characterization techniques often cannot be applied. A information gap therefore exists to characterize these materials and in particular the influence of adding actinides, such as uranium (U) and plutonium (Pu), on the properties of the melts. While modeling can close some of these gaps, experimental data to benchmark these models is scarce. This proposal closes this gap by providing data on the pair-distribution function of the melts as a function of temperature and composition, including U and Pu. Assembling a team of experts in neutron characterization and molten salts and building on Los Alamos's unique capability to handle actinide-bearing samples, not available at other user facilities, we propose to use neutron pair-distribution function (PDF) analysis to characterize the local structure of molten salts in situ.

Publications

Presentation Slides

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)

Accelerated Development of Additively Manufactured Uranium Oxide (UO2) Fuels for Geometries Avoiding Fuel Lifetime-limiting Irradiation Swelling Using Bulk Neutron Characterization

Bjorn Clausen
20200749DI

Project Description

In nuclear reactor environments, increasing burnup results in swelling of nuclear fuels due to the formation of fission gas bubbles and accumulation of solid fission products, limiting the achievable burnup and therefore the fuel economy. The use of fuel geometries other than sheets or cylinders can enhance geometrical stability at lower overall densities, which can mitigate the swelling, especially at ultra-high burnups. However, conventional fabrication techniques, especially for ceramic uranium dioxide (UO2) fuels, precluded development of such fuel forms. In recent years, significant development of advanced manufacturing technologies allows novel designs to overcome these limitations and fabricate fuel geometries that accommodate swelling much better, hence enabling higher burnup and therefore improve the economy of nuclear power generation. This project will leverage Los Alamos' unique characterization capabilities to advance this development, enabled by the pulsed neutron source at the Los Alamos Neutron Science Center, the high-energy X-ray computer tomography within the Non-Destructive Testing and Evaluation group, as well as existing Los Alamos infrastructure to handle nuclear materials. The non-destructive advanced characterization tools employed will for the first time give a complete picture of density and microstructure variations at the component length scale that can be used to optimize the manufacturing process.

Beyond the Hugoniot: Dynamic Strength and Damage in Polymers

Jennifer Jordan
20200083DI

Project Description

Simulations of the dynamic response of polymers require coupled equation of state, strength and damage models, which have historically not been implemented in hydrocodes because the polymer strength was not seen as relevant in the simulation. In this project, we will investigate whether polymer strength plays a role in dynamic experiments and whether variations in that strength result in measurable differences in an integrated experiment. This understanding will allow us to develop relevant, mesoscale informed polymer models providing the ability to accurately predict complex experiments.

Technical Outcomes

The project team characterized the quasi-static elastic properties and strength of polyethylene, contributed to the understanding of properties and structure under static and dynamic high pressure, compared existing models with a relevant explosively loaded experiment, and explored connections between material properties and structure. The elastic properties and strength of polyethylene were found to vary 2-2.5x depending on the underlying structure. Additionally, existing models were shown to lack prediction for experimental data.

Publications

Journal Articles

Jordan, J. L., R. L. I. Rowland, J. J. Greenhall, E. K. Moss, R. C. Huber, E. C. Willis, C. Kenney-Benson, B. D. Bartram, B. Sturtevant and R. Hrubiak. Elastic Properties of Polyethylene from High Pressure Sound Speed Measurements. Submitted to *Polymer*. (LA-UR-20-25115)

Jordan, J. L. and D. T. Casem. Understanding Calibration and Error Propagation in Longitudinal and Lateral Manganin Gauge Shock Experiments. 2020. *Journal of Dynamic Behavior of Materials*. (LA-UR-20-23748 DOI: 10.1007/s40870-020-00255-7)

Presentation Slides

Jordan, J. L. Elastic Properties of Polyethyene from High Pressure Sound Speed Measurements. Presented at *C2 Weekly Meeting*, Los Alamos, New Mexico, United States, 2020-08-19 - 2020-08-19. (LA-UR-20-26364)

Jordan, J. L., R. C. Huber, B. Sturtevant, R. L. I. Rowland, E. K. Moss, J. J. Greenhall and D. M. Dattelbaum. Dynamic Strength in Polymers. Presented at *American Physical Society March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21961)

Hybrid Materials Architectures for Quantum Information Science

Jinkyoung Yoo
20200672DI

Project Description

Relentless progress in quantum information science, realized by demonstration of applications based on quantum phenomena, will encounter fundamental limitations due to lack of diverse materials that can be utilized for various quantum technologies. Observation of quantum phenomena at cryogenic temperature and weak interaction between quantum materials and external control knobs have blocked exploration of quantum sciences in materials. Furthermore, currently available quantum materials are not suitable for scalable and deployable quantum systems. This project aims at developing materials strategies overcoming current limitations of physical implementation of quantum information science. The key approaches are synthesis of high-quality quantum materials, integration of different quantum materials in an architecture, in-depth characterizations of quantum materials heterostructures at multi-scales, and thorough understanding of mechanisms of quantum materials synthesis. Performing this project opens up ways of quantum materials studies through offering novel quantum materials, such as topological superconducting materials, two-dimensional nanomagnets, and enhanced multi-coupled electronic materials. Moreover, study on architectures composed of quantum materials will bring essential knowledge on interface in quantum systems because processes governing quantum system's functionalities, which are injection (e.g. electrodes), manipulation (e.g. active channel of transport), and transduction (e.g. interconnects) of quantum information carriers, occur across interfaces of quantum materials.

Technical Outcomes

Two hybrid materials for error-tolerant quantum information processing were demonstrated. A hybrid architecture composed of conventional semiconductors (silicon and germanium) and metallic ceramic showed basic properties required for error-tolerant quantum computer. A newly synthesized magnetic material also showed magnetic properties useful for quantum computer. The new magnetic material can be prepared in the form of a few atomically thin layers. The ultimate thinness enables to fabricate integrated and miniaturized information processing system.

Publications

Journal Articles

*Liu, C., H. Tsai, W. Nie, D. J. Gosztola and X. Zhang. Direct Spectroscopic Observation of the Hole Polaron in Lead Halide Perovskites. 2020. *The Journal of Physical Chemistry Letters*. **11** (15): 6256-6261. (LA-UR-20-24148 DOI: 10.1021/acs.jpclett.0c01708)

Sirica, N. S., P. Orth, M. Scheurer, Y. Dai, M. C. Lee, P. Padmanabhan, L. M. T. Mix, L. X. Zhao, G. Chen, B. Xu, R. Yang, B. Shen, C. C. Lee, H. Lin, S. A. Trugman, J. Zhu, 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. Submitted to *Nature Materials*. (LA-UR-20-23580)

Atomic Armor Protecting Plutonium

Doinita Neiner
20200748DI

Project Description

The “Atomic Armor Protecting Plutonium" Focused Response project is aimed at a new concept to address plutonium metal oxidation or corrosion, namely the use of Atomic Armor in the form of graphene or graphene oxide coatings. Plutonium metal is a highly reactive metal that rapidly oxidizes. Oxidation or corrosion can be extremely detrimental to a process flow stream and product output within a manufacturing environment, can significantly influence the requirements for handling and storage of plutonium materials, and can impact the use of plutonium materials in a variety applications or scientific studies. This project is a small-scale, cutting-edge, high-risk and high pay-off project, that if successful will have applications across several plutonium science and technology areas. In this project, a set of systematic experiments will be performed to evaluate the oxidation or corrosion protection of graphene and graphene oxide metallic plutonium surfaces across a variety of typical manufacturing, storage, and handling environments.
If found to be successful, graphene or graphene oxide coatings will provide an alternate method to protect plutonium against oxidation and corrosion. This would have direct ties to not only actinide science, research and technology but would show particular relevance to the plutonium manufacturing mission.

Technical Outcomes

This project developed a graphene oxide (GO) membrane and a sample preparation method for encapsulation; characterization of the samples in progress. Four experiments have been performed, a leak test with helium (He), two corrosive gasses tests and a radiation damage test. The corrosion experiments look promising in that the GO membrane acts as a gas barrier, protecting the metal surface from corrosion.

Formation of Actinide Amalgams from Ionic Liquids

George Goff
20200750DI

Project Description

This project aims to lay the ground work for new technologies that could replace the high temperature molten salts used in conventional electrochemical processes for special nuclear material production. This would significantly increase the safety of these processes (enable low temperature operations), eliminate highly corrosive halide molten salts, and significantly decrease the waste effluents. Ionic liquids (ILs) possess unique physical properties that make them particularly attractive for a number of actinide applications. This project proposes to form mercury amalgams of uranium (U), plutonium (Pu), and neptunium (Np) through deposition of these actinides from ionic liquids using electrical energy. Such amalgams are of interest since mercury can be evaporated to leave pure actinide metals. Understanding Pu chemistry is a core mission at Los Alamos. This could serve as the basis for enabling small-scale sample prep for Pu metal samples used by the Office of Experimental Sciences and other programmatic and basic science programs across the Lab. Various isotopic separation processes require metal targets (ion separation capability being developed for Pu-242 production) or metal products, and this could be an enabling technology. There are only a handful of manuscripts on transuranic chemistry in ILs, and no reports of amalgam or metal formation.

Technical Outcomes

This project successfully demonstrated the production of uranium amalgams from ionic liquids using two different production routes. The first involved electroreduction of Uranium from an ionic liquid using a liquid mercury electrode, and the second route used a non-electrochemical metathesis route using a sodium amalgam. The team also synthesized several novel anhydrous starting materials for solubilizing uranium into ionic liquids and developed the safety basis to extend this work to transuranic elements.

Ultrasonic Filtration: A Revolutionary Technology for Hydroxide Precipitation

James Coons
20200754DI

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, 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. Therefore, the key initial step in the pathway to defining, developing and building this innovative hydroxide precipitation process is this Proof of Principle study.

Technical Outcomes

A bench-top ultrasonic filter demonstration successfully removed iron hydroxide from an aqueous suspension. Hindered settling was observed indicating improvement is possible with pH control. These results demonstrate the clear potential of this technology to revolutionize hydroxide precipitation processing at TA-55 by alleviating fundamental constraints, dramatically reducing radiation dose and physical demands to operators, and improving the caustic glovebox atmospheres that contribute to equipment corrosion and shortened lifetimes.

Theory and Computation on Quantum Systems

Angel Garcia
20190495CR

Project Description

This project addresses fundamentals of the electronic properties of materials, from actinides to photovoltaics, with emphasis on computational algorithms. We will apply concepts and algorithms of quantum computation to (1) understand the electronic structure of materials from complex correlated systems (2) explore novel functionality in topologically protected states, and (3) Explore new quantum computing algorithms to solve optimization problems in quantum computers and/or annealers. This work has relevance in developing new materials for energy applications, modeling and predicting properties of f-electron matter, including plutonium, for National Nuclear Security Administration mission objectives, and developing materials for quantum computing applications.

Publications

Journal Articles

Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihal\xc3\xa1k. Near-gathering of energy-constrained mobile agents. 2020. *Theoretical Computer Science*. (LA-UR-19-23906 DOI: 10.1016/j.tcs.2020.10.008)

Beckey, J., A. Sone, M. V. S. Cerezo de la Roca and P. J. Coles. Variational Quantum Fisher Information Estimation. Submitted to *Quantum*. (LA-UR-20-28328)

Bilkis, M., M. V. S. Cerezo de la Roca, G. Verdon, P. J. Coles and L. Cincio. A semi-agnostic ansatz with variable structure for quantum machine learning. Submitted to *Quantum*. (LA-UR-21-22040)

Bravo-Prieto, C., R. LaRose, M. V. S. Cerezo de la Roca, Y. Subasi, L. Cincio and P. J. Coles. Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems. Submitted to *arXiv*. (LA-UR-19-29101)

Cerezo, M., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation. 2020. *Quantum*. **4**: 248. (LA-UR-19-25585 DOI: 10.22331/q-2020-03-26-248)

Fontana, E., M. V. S. Cerezo de la Roca, A. T. Arrasmith, I. Runnger and P. J. Coles. Optimizing parameterized quantum circuits via noise-induced breaking of symmetrie. Submitted to *Quantum*. (LA-UR-20-29359)

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)

Ghosh, D., A. J. Neukirch and S. Tretiak. Light Emission in 2D Bromide Perovskites : Spacer Cations Matter. Submitted to *Nano Letters*. (LA-UR-19-31189)

Ghosh, D., D. Acharya, L. Pedesseau, C. Katan, J. Even, S. Tretiak and A. J. Neukirch. Charge Carrier Dynamics in Two-Dimensional Lead Iodide Perovskites: Dion-Jacobson vs. Ruddlesden-Popper Phases. Submitted to *ACS Nano*. (LA-UR-20-25290)

*Ghosh, D., D. Acharya, L. Zhou, W. Nie, O. V. Prezhdo, S. Tretiak and A. J. Neukirch. Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. 2019. *The Journal of Physical Chemistry Letters*. **10** (17): 5000-5007. (LA-UR-19-26501 DOI: 10.1021/acs.jpclett.9b02020)

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Theoretical and Experimental Materials Science

Filip Ronning
20190497CR

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.

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Properties, Theory, and Measurements for Understanding the Function of Heavy Elements

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20180474CR

Project Description

The study of heavy elements continues to be essential to the United States and central to the missions of the Department of Energy and its National Nuclear Security Administration (NNSA) laboratories, including nuclear weapons, global security, environmental restoration, and radioactive waste management. Of real concern is the recognition that academic degree programs and research opportunities in heavy-element science are small so that the field is becoming subcritical at a crucial time for our nation. Research performed by competitively selected Seaborg supported postdoctoral Fellows and students in nuclear science has provided exceptional return on investment in both science and acquisition of new hires.

Technical Outcomes

The Glenn T. Seaborg Institute Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project has advanced heavy element and actinide science by targeting Los Alamos mission imperatives from 2018 to 2020. During implementation this project supported 34 2-year postdoctoral fellows' research and 122 publications, 53 graduate (GRA) summer student research fellowships, numerous workshops and integrated educational and career development opportunities, and new initiatives such as Rapid Response Projects supporting LANL actinide mission.

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Baker, J. L. Material Properties at Extreme Pressures and Temperatures. . (LA-UR-20-26623)

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Pagano, J. K. An inorganic chemistry course as research: My experience with CUREs. Presented at *ACS National Meeting & Exposition Fall 2019*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-27302)

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Lai, Y. Tuning the ferromagnetic tri-critical point and quantum critical point in Ce(Pd1-xNix)2P2 under high magnetic fields. Presented at *LANL 2018 Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-25490)

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Nuclear and Particle Futures

A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility

Mark Schmitt
20180051DR

Project Description

We will investigate key aspects of achieving ignition using direct laser drive of a triple shell implosion system. The achievement of fusion in the laboratory is a grand challenge problem whose solution would be recognized worldwide and advance research in both fusion energy and weapons science. If successful, a completely new venue for experiments to understand and explore the conditions of ignition in the laboratory would be born.

Publications

Journal Articles

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*Molvig, K., M. J. Schmitt, R. Betti, E. M. Campbell and P. McKenty. Stable and confined burn in a Revolver ignition capsule. 2018. *Physics of Plasmas*. **25** (8): 82708. (LA-UR-18-23353 DOI: 10.1063/1.5037224)

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Nucleosynthesis Probes of Cosmic Explosions

Christopher Fryer
20190021DR

Project Description

Multi-physics modeling, combining transport, nuclear physics, and hydrodynamics all play an important role in a range of problems of national interest. This project brings together both physics experts and computational scientists to study the multi-physics problem surrounding the emission of from the merger of two neutron stars. The physics components and the numerical methods used to combine these physics components will develop techniques Los Alamos scientists will be able to use throughout the Advanced Simulation and Computing (ASC) program.

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The Neutron Electric Dipole Moment as a Gateway to New Physics

Takeyasu Ito
20190041DR

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.

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Convincing Search for Sterile Neutrinos at Lujan

Richard Van De Water
20190098DR

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 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.

Publications

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A New Era of Nuclear Physics at the Electron-Ion Collider

Ivan Vitev
20200022DR

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.

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High-Gradient, High-Efficiency Radio-frequency (RF) Structures: Smart Design Based on Informed Break-down Suppression

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20200057DR

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 US-based C-band test accelerator site.

Publications

Journal Articles

Chylek, P., C. Folland, J. Klett and M. K. Dubey. Arctic Amplification and Arctic temperature anomaly: Observed and simulated by thirteen CMIP6 climate models. Submitted to *Quaterly Journal of Royal Meteorological Society*. (LA-UR-21-21658)

Reports

Perez, D. IC report: Materials design for high-gradient RF structures. Unpublished report. (LA-UR-21-21989)

Presentation Slides

Krawczyk, F. L. C-band – The Big Picture. Presented at *LANL 2020 Engineering Capability Review*, Los Alamos, New Mexico, United States, 2020-09-09 - 2020-09-11. (LA-UR-20-26179)

Krawczyk, F. L., E. I. Simakov, D. Perez, G. Wang, A. W. Garmon, M. F. Kirshner, J. T. I. Bradley, E. Nanni, S. Tantawi, D. Gamzina, J. B. Rosenzweig and A. Fukasawa. Technology Development of High-gradient C-band based Accelerators. Presented at *Linear Collider Workshop LCWS 2019*, Sendai, Japan, 2019-10-28 - 2019-11-01. (LA-UR-19-30794)

I. Lewellen, J. W., E. I. Simakov, T. Tajima and P. Pizzol. Status of Cryo Work at LANL. . (LA-UR-21-21926)

Perez, D. C-Band materials modeling efforts at LANL. . (LA-UR-20-28389)

Schneider, M. E., E. Jevarjian, J. Shao, T. Posos, T. Nikhar, W. Lui and S. V. Baryshev. Demonstration of Ampere-class Field Emission Cathodes Operating at 100 MV/M and Excess of Child-Langmuir Law. Presented at *Advanced accelerator concepts 2020: seminar series*, online, California, United States, 2021-01-13 - 2021-01-13. (LA-UR-21-20177)

Schneider, M. E., E. Jevarjian, J. Shao and S. V. Baryshev. FEbeam: A Comprehensive Field Emission Data Processing for Field Emission and Breakdown Analysis in RF Environment. Presented at *9th International Workshop on Mechanisms of Vacuum Arcs (MeVArc 2021)*, online, Switzerland, 2021-03-08 - 2021-03-12. (LA-UR-21-22291)

Schneider, M. E., R. L. Fleming, E. Jevarjian, E. I. Simakov, S. V. Baryshev, D. V. Gorelov and J. W. I. Lewellen. FEbreak: A Comprehensive Diagnostic and Automated Conditioning Interface for Analysis of Breakdown and Dark Current Effects. Presented at *9th International Workshop on Mechanisms of Vacuum Arcs (MeVArc 2021)*, online, Switzerland, 2021-03-08 - 2021-03-12. (LA-UR-21-22292)

Predictive Understanding of Device Performance Through Innovative Measurement, Modeling, and Simulation on Radiochemical Dosimeters

Paul Koehler
20200108DR

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

Presentation Slides

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)

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., P. E. Koehler, A. Stamatopoulos, A. J. Couture, B. J. DiGiovine and J. L. Ullmann. First DICER results from 191Ir and 193Ir. Presented at *LDRD DR Project Appraisal (20200108DR Koehler)*, Los Alamos, New Mexico, United States, 2020-12-10 - 2020-12-10. (LA-UR-20-30110)

Deepening Los Alamos National Laboratory's Neutrino Legacy

Steven Elliott
20180038DR

Project Description

This project will develop and maintain several important capabilities for the Laboratory. These include isotope identification skills defined by both experimental and analytical techniques; the development of radiation detection skills and the analysis of arrays of radiation detectors; the development of radio-pure materials; and the theoretical and large-scale computational analysis of phenomena in hadronic physics and in complex nuclei and novel double beta decay physics. This proposal paves the way and reduces risk for the Department of Energy's plan for a 1000-kg project and enhances Los Alamos' reputation as a scientific leader. This program has had a large impact on recruitment at the laboratory. Of the 15 completed post-docs from the last decade on the Weak Interactions team, 5 are now staff scientists at LANL and 5 are faculty at Universities. The remaining are working in industry or other laboratories. Past Theory postdocs at the lab are employed within the laboratory, as faculty at universities, or continue as postdocs at universities or laboratories.

Technical Outcomes

This project developed a second vendor for enriched stable isotope and demonstrated the utility of detectors made from this material. These developments will significantly reduce risk and cost for a future experiment based on Germanium-76. The lattice quantum chromodynamics (QCD) effort established the importance of including lower energy intermediate neutron-pion (Nπ) states in the calculation of all nucleon matrix elements. In the effective field theory the recognition of the new leading order operator to double beta decay was critical.

Publications

Journal Articles

*Alvis, S. I., I. J. Arnquist, F. T. I. Avignone, A. S. Barabash, C. J. Barton, V. Basu, F. E. Bertrand, B. Bos, M. Busch, M. Buuck, T. S. Caldwell, Y. -. D. Chan, C. D. Christofferson, P. -. H. Chu, M. Clark, C. Cuesta, J. A. Detwiler, Y. Efremenko, H. Ejiri, S. R. Elliott, T. Gilliss, G. K. Giovanetti, M. P. Green, J. Gruszko, I. S. Guinn, V. E. Guiseppe, C. R. Haufe, R. J. Hegedus, L. Hehn, R. Henning, D. H. Aguilar, E. W. Hoppe, M. A. Howe, M. F. Kidd, S. I. Konovalov, R. T. Kouzes, A. M. Lopez, R. D. Martin, R. Massarczyk, S. J. Meijer, S. Mertens, J. Myslik, G. Othman, W. Pettus, A. Piliounis, A. W. P. Poon, D. C. Radford, J. Rager, A. L. Reine, K. Rielage, N. W. Ruof, B. Shanks, M. Shirchenko, D. Tedeschi, R. L. Varner, S. Vasilyev, B. R. White, J. F. Wilkerson, C. Wiseman, W. Xu, E. Yakushev, C. -. H. Yu, V. Yumatov, I. Zhitnikov and B. X. Zhu. Search for neutrinoless double- decay in with 26 kg\xc2\xa0yr of exposure from the Majorana Demonstrator. 2019. *Physical Review C*. **100** (2): 025501. (LA-UR-19-20700 DOI: 10.1103/PhysRevC.100.025501)

*Alvis, S. I., I. J. Arnquist, F. T. I. Avignone, A. S. Barabash, C. J. Barton, V. Basu, F. E. Bertrand, B. Bos, M. Buuck, T. S. Caldwell, Y. -. D. Chan, C. D. Christofferson, P. -. H. Chu, C. Cuesta, J. A. Detwiler, H. Ejiri, S. R. Elliott, T. Gilliss, G. K. Giovanetti, M. P. Green, J. Gruszko, I. S. Guinn, V. E. Guiseppe, C. R. Haufe, R. J. Hegedus, L. Hehn, R. Henning, D. H. Aguilar, E. W. Hoppe, M. A. Howe, K. J. Keeter, M. F. Kidd, S. I. Konovalov, R. T. Kouzes, A. M. Lopez, R. D. Martin, R. Massarczyk, S. J. Meijer, S. Mertens, J. Myslik, G. Othman, W. Pettus, A. Piliounis, A. W. P. Poon, D. C. Radford, J. Rager, A. L. Reine, K. Rielage, N. W. Ruof, B. Shanks, M. Shirchenko, D. Tedeschi, R. L. Varner, S. Vasilyev, B. R. White, J. F. Wilkerson, C. Wiseman, W. Xu, E. Yakushev, C. -. H. Yu, V. Yumatov, I. Zhitnikov and B. X. Zhu. Multisite event discrimination for the majorana demonstrator. 2019. *Physical Review C*. **99** (6): 065501. (LA-UR-19-20305 DOI: 10.1103/PhysRevC.99.065501)

*Alvis, S. I., I. J. Arnquist, F. T. I. Avignone, A. S. Barabash, C. J. Barton, V. Basu, F. E. Bertrand, B. Bos, V. Brudanin, M. Busch, M. Buuck, T. S. Caldwell, Y. Chan, C. D. Christofferson, P. Chu, C. Cuesta, J. A. Detwiler, Y. Efremenko, H. Ejiri, S. R. Elliott, T. Gilliss, G. K. Giovanetti, M. P. Green, J. Gruszko, I. S. Guinn, V. E. Guiseppe, C. R. Haufe, R. J. Hegedus, L. Hehn, R. Henning, D. H. Aguilar, E. W. Hoppe, M. A. Howe, K. J. Keeter, M. F. Kidd, S. I. Konovalov, R. T. Kouzes, A. M. Lopez, R. D. Martin, R. Massarczyk, S. J. Meijer, S. Mertens, J. Myslik, G. Othman, W. Pettus, A. Piliounis, A. W. P. Poon, D. C. Radford, J. Rager, A. L. Reine, K. Rielage, N. W. Ruof, B. Shanks, M. Shirchenko, D. Tedeschi, R. L. Varner, S. Vasilyev, B. R. White, J. F. Wilkerson, C. Wiseman, W. Xu, E. Yakushev,

C. Yu, V. Yumatov, I. Zhitnikov and B. X. Zhu. Search for trinucleon decay in the Majorana Demonstrator. 2019. *Physical Review D*. **99** (7): 072004. (LA-UR-18-31257 DOI: 10.1103/PhysRevD.99.072004)

*I. Avignone, F. T. and S. R. Elliott. The Search for Double Beta Decay With Germanium Detectors: Past, Present, and Future. 2019. *Frontiers in Physics*. **7**: 6. (LA-UR-18-30325 DOI: 10.3389/fphy.2019.00006)

*Carlson, J. A., A. Lovato, S. Gandolfi, N. Rocco and R. Schiavilla. Study of (v_l, l) and (nubar, l+) Inclusive Scattering in 12C: Confronting the MiniBooNE and T2K CCQE Data. 2020. *Physical Review X*. **10** (3): 31068. (LA-UR-20-22484 DOI: 10.1103/PhysRevX.10.031068)

Chu, P., S. R. Elliott, I. w. Kim, R. Massarczyk, S. J. Meijer, K. R. Rielage, B. White, X. B. Zhu and M. J. Stortini. ADC Nonlinearity Correction for the Majorana Demonstrator. Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-20-21663)

Chu, P., T. R. Edwards, S. R. Elliott, I. w. Kim, R. Massarczyk, S. J. Meijer, K. R. Rielage, B. Sayki and M. J. Stortini. \xce \xb1-event Characterization and Rejection in Point-Contact HPGe Detectors. Submitted to *Physical Review C*. (LA-UR-20-24209)

Elliott, S. R., M. Gold, K. R. Rielage, R. Massarczyk, N. C. Mcfadden, D. Fields, D. Loomba and R. Gibbons. Large-Scale, Precision Xenon Doping of Liquid Argon. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-20-23118)

Gupta, R., b. Joo, T. Bhattacharya, B. Yoon, S. Park, S. Mondal, F. winter and Y. C. Jang. Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD. Submitted to *Physical Review D*. (LA-UR-21-20526)

*Jang, Y., R. Gupta, B. Yoon and T. Bhattacharya. Axial Vector Form Factors from Lattice QCD that Satisfy the PCAC Relation. 2020. *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. **124** (7): 072002. (LA-UR-19-29302 DOI: 10.1103/PhysRevLett.124.072002)

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Massarczyk, R., R. Schwengner, D. Bemmerer, R. Beyer, M. Bhike, B. A. Brown, M. Butterling, V. Derya, M. Dietz, F. Fiedler, A. Frotscher, U. Gayer, A. Hartmann, A. R. Junghans, T. Koegler, F. Krishichayan, F. Ludwig, B. Lutz, H. Pai, K. Roemer, M. Takacs, T. Szucs, W. Tornow and A. Wagner. Electric and magnetic dipole strength in 54Fe. Submitted to *PRC*. (LA-UR-20-22566)

Massarczyk, R., S. R. Elliott, K. R. Rielage, D. Fields, R. Gibbons, M. Gold, J. Thomas and N. McFadden. A Kinetic Model for Xenon-Doped Liquid Argon Scintillation Light. Submitted to *Physical Review C*. (LA-UR-20-27430)

Mereghetti, E., V. Cirigliano, W. G. Dekens, J. de Vries, M. L. Graesser, S. Pastore, M. Piarulli, U. Van Kolck and R. B. Wiringa. A renormalized approach to neutrinoless double beta decay. Submitted to *Physical Review C*. (LA-UR-19-26002)

*Mondal, S., R. Gupta, S. Park, B. Yoon, T. Bhattacharya and H. Lin. Moments of nucleon isovector structure functions in 2 + 1 + 1-flavor QCD. 2020. *Physical Review D*. **102** (5): 054512. (LA-UR-20-23801 DOI: 10.1103/PhysRevD.102.054512)

*Wang, X. B., A. C. Hayes, J. Carlson, G. X. Dong, E. Mereghetti, S. Pastore and R. B. Wiringa. Comparison between variational Monte Carlo and shell model calculations of neutrinoless double beta decay matrix elements in light nuclei. 2019. *Physics Letters B*. **798**: 134974. (LA-UR-19-25587 DOI: 10.1016/j.physletb.2019.134974)

Conference Papers

Gupta, R., S. Park, T. Bhattacharya, Y. Jang, J. Bailey, B. Choi, H. Jeong, S. Jwa, S. Lee, W. Lee, J. Pak and J. Leem. Update on B \xe2\x86\x92 D\xe2\x88\x97l\xce\xbd form factor at zero-recoil using the Oktay-Kronfeld action. Presented at *The 36th Annual International Symposium on Lattice Field Theory - LATTICE2018*. (East Lansing, Michigan, United States, 2018-07-22 - 2018-07-28). (LA-UR-19-20196)

Reports

Gupta, R., T. Bhattacharya, J. A. Carlson, S. Gandolfi, B. Yoon, S. Park, S. Mondal, S. Pastore, H. W. Lin and Y. Jang. Snowmass2021 - Letter of Interest Theoretical predictions of Neutrino-nucleus Interactions. Unpublished report. (LA-UR-20-26766)

Massarczyk, R. Radioactive Sources for LEGEND-200 at LANL. Unpublished report. (LA-UR-21-21754)

Presentation Slides

Bhattacharya, T. Nucleon Matrix Elements for HEP and NP. . (LA-UR-20-26716)

Bhattacharya, T. Lattice Gauge Theory for High Energy Physics: Fundamental Symmetries brief. Presented at *Snowmass 2021 Community Planning Meeting*, Online, Illinois, United States, 2020-10-05 - 2020-10-07. (LA-UR-20-27911)

Bhattacharya, T. Calculating neutron properties to look for new physics. . (LA-UR-21-22554)

Elliott, S. R. Future of Double Beta Decay. Presented at *3rd Conference on Science at the Sanford Underground Research Facility*, Rapid City, South Dakota, United States, 2019-05-15 - 2019-05-17. (LA-UR-19-24356)

Elliott, S. R. LEGEND: The Large Enriched Germanium Experiment for Neutrinoless Double-Beta Decay. Presented

at *APS April Meeting*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23033)

Elliott, S. R. Future Double Beta Experiments. Presented at *Heraeus Seminat*, Bad Honnef, Germany, 2019-07-08 - 2019-07-11. (LA-UR-19-26621)

Elliott, S. R. LEGEND. Presented at *SNOLAB Future Projects Workshop*, Sudbury, Canada, 2019-07-15 - 2019-07-17. (LA-UR-19-26849)

Elliott, S. R. Update on Double Beta Decay Experiments. Presented at *DBD Topical Nuclear Theory Collaboration Spring 2020 Meeting*, remote, New Mexico, United States, 2020-05-28 - 2020-05-29. (LA-UR-20-23864)

Gupta, R. Probing novel phenomena with protons and neutrons using Lattice QCD at LANL:. . (LA-UR-20-22643)

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Massarczyk, R. LEGEND. Presented at *"Double beta decay and underground science" (DBD18)"*, Hawaii Island, Hawaii, United States, 2018-10-21 - 2018-10-21. (LA-UR-18-29731)

Massarczyk, R. From MAJORANA to LEGEND. Presented at *Neutrino Nuclear Responses 2019 (NNR19) for Double Beta Decays and Astro Neutrinos*, Osaka, Japan, 2019-05-08 - 2019-05-08. (LA-UR-19-24026)

Massarczyk, R. Status and Recent Results of the Majorana Demonstrator. Presented at *9th International Conference on New Frontiers in Physics*, online, New Mexico, United States, 2020-09-05 - 2020-09-05. (LA-UR-20-26800)

Massarczyk, R., I. w. Kim, S. J. Meijer, S. R. Elliott and P. Chu. Status of LEGEND : Progress on LEGEND-200 & Outlook towards ton-scale. Presented at *APS virtual meeting*, Washington, District Of Columbia, United States, 2020-04-18 - 2020-04-18. (LA-UR-20-22909)

Posters

Massarczyk, R., S. R. Elliott, S. J. Meijer, I. w. Kim and R. Henning. Search for Beyond the Standard Model physics with LEGEND-1000. Presented at *Neutrino 2020 (virtual) organized by Fermilab*, Batavia, Illinois, United States, 2020-06-22 - 2020-06-22. (LA-UR-20-23958)

Quantifying Effects of Magnetic Fields for Inertial Confinement Fusion (ICF)/ High-Energy-Density (HED) Plasmas with Instabilities and Turbulence

Kirk Flippo
20180040DR

Project Description

This project helps address energy security and stockpile stewardship challenges by helping to understand and quantify the roles of self-generated magnetic fields in Inertial Confinement Fusion (ICF) implosions like those at the National Ignition Facility (NIF).

Technical Outcomes

The experimental objective to characterize the effects of magnetic fields in inertial confinement fusion (ICF)-relevant plasmas was achieved by carrying out experiments with a simple geometry yet capturing key magnetized turbulent processes and was shown to produce fields on the order of 10 tesla (T). The theoretical objective of developing a validated model for field generation and amplification was achieved with several new discoveries, and showed that to accurately understand these fields one must include all the extended magnetohydrodynamic drive (MHD) terms.

Publications

Journal Articles

Li, H. Signatures of Alfv \xcc\x81en-mode and Slow-mode Waves and Non-Propagating Structures in 3D Compressive MHD Turbulence. Submitted to *Astrophysical Journal*. (LA-UR-18-30429)

*Lu, Y., H. Li, K. A. Flippo, K. V. Kelso, A. S. Liao, S. Li and E. P. Liang. MPRAD: A Monte Carlo and ray-tracing code for the proton radiography in high-energy-density plasma experiments. 2019. *Review of Scientific Instruments*. **90** (12): 123503. (LA-UR-19-27741 DOI: 10.1063/1.5123392)

*Lu, Y., P. Tzeferacos, E. Liang, R. K. Follett, L. Gao, A. Birkel, D. H. Froula, W. Fu, H. Ji, D. Lamb, C. K. Li, H. Sio, R. Petrasso and M. S. Wei. Numerical simulation of magnetized jet creation using a hollow ring of laser beams. 2019. *Physics of Plasmas*. **26** (2): 22902. (LA-UR-19-20212 DOI: 10.1063/1.5050924)

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Sadler, J. D., H. Li and K. A. Flippo. Magnetic field generation from composition gradients in inertial confinement fusion fuel. Submitted to *Philosophical Transactions of the Royal Society A. Mathematical, Physical and Engineering Sciences*. (LA-UR-20-22152)

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Sadler, J. D. and H. Li. Thermomagnetic instability of plasma composition gradients. Submitted to *Physics of Plasmas*. (LA-UR-20-26924)

Reports

Rasmus, A. M. Shock driven discrete vortex growth on oblique interfaces. Unpublished report. (LA-UR-18-26572)

Presentation Slides

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Flippo, K. A. Shock-driven magnetic field generation in ICF relevant plasmas. Presented at *Kinetic Effects in ICF Workshop*, Santa Fe, New Mexico, United States, 2018-05-22 - 2018-05-25. (LA-UR-18-24503)

Flippo, K. A. High Energy Density Hydrodynamics and ICF Experiments at Los Alamos National Lab. . (LA-UR-19-26212)

Flippo, K. A. HEDB - High Energy Density with B-fields research for ICF and Lab-Astro at LANL: An Overview. Presented at *American Physical Society Division of Plasma Physics*, online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-29327)

Flippo, K. A., A. M. Rasmus, C. Y. Fiedler Kawaguchi, B. J. Tobias, T. Desjardins, E. C. Merritt, C. Di Stefano, F. W. Doss, S. Palaniyappan, J. P. Sauppe, T. N. Archuleta, R. P. Gonzales, V. A. Garcia, D. W. Schmidt, A. Strickland, D. H. Barnak and C. C. Kuranz. Developing New X-ray Diagnostic Methods for HED Hydrodynamic Experiments. Presented at *61st American Physical Society Division of Plasma Physics Meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30706)

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Li, H. Modeling and Experiments of Turbulent Flows with Applications to Astrophysics and Space Physics. . (LA-UR-18-30383)

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Sadler, J. D., H. Li, K. A. Flippo and Y. Lu. Two-dimensional kinetic simulations of hot-spot ablator mix. Presented at *American Physical Society division of plasma physics conference*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30614)

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Production of Shaped Electron Bunches with Diamond Field Emitter Array Cathodes

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20180078ER

Project Description

This project has the potential to advance the diamond field emitter array (DFEA) cathode technology and make it suitable for a number of national security applications that require high current, high power electron beams. This includes compact accelerators for warfighter support (e.g. small weaponized free-electron lasers), active interrogation, environmental remediation, and multi-megawatt X-ray sources. DFEAs present the most natural means of producing very high current electron bunches: they produce electron beams from the tips of diamond pyramids that can be fabricated and arranged in customized arbitrary patterns to suit the particular application, they generate a very stable and robust electron beam, and they produce the extremely high current densities that are necessary for obtaining multi-nano-Coulomb bunches.

Publications

Journal Articles

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Simakov, E. I., H. L. Andrews, C. Huang, T. J. T. Kwan, D. Kim, J. W. I. Lewellen, K. Nichols and V. Pavlenko. High current field emission electron sources for linear colliders and RF source applications. Presented at *Particle Physics Community Planning Exercise (Snowmass 2021)*. (Seattle, Washington, United States, 2021-07-11 - 2021-07-11). (LA-UR-20-26499)

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Posters

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Schneider, M. E., D. Kim, K. Nichols, H. L. Andrews, E. I. Simakov, E. Jevarjian, S. Baryshev and J. Shao. Application of FEgen for Guided Development of Transversely Shaped Beams using Field Emission Arrays. Presented at *AAC Seminar Series 2020*, Virtual, California, United States, 2020-11-18 - 2021-01-06. (LA-UR-20-29454)

Schneider, M. E., E. Jevarjian, J. Shao, T. Posos, T. Nikhar, W. Lui and S. V. Baryshev. Developed and experimentally vetted ampere-class field emission cathode (FEC) operated up to 100 MV/m and Beyond Child Langmuir. Presented at *ACC Seminar Series*, Digital, California, United States, 2020-11-18 - 2021-01-06. (LA-UR-20-29445)

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Pinning Down the Neutrino-proton Process Importance in Heavy Element Production via Reaction Studies on Radioactive Nickel-56

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20180228ER

Project Description

The entire project effort, from radioactive sample production at the Isotope Production Facility to performing neutron-induced reactions at Los Alamos Neutron Science Center, can be only performed at Los Alamos National Laboratory in the US. The project results will extend to the study of nuclear reactions on radioactive samples, directly related to NNSA missions, including radiochemical detector analysis, device diagnostics, and other areas. Through this project we will improve our understanding of nuclear reaction mechanisms with mission relevance.

Publications

Journal Articles

*Kim, H. I., H. Y. Lee, T. Kawano, A. Georgiadou, S. A. Kuvin, L. Zavorka and M. W. Herman. New evaluation on angular distributions and energy spectra for neutron-induced charged-particle measurements. 2020. *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. **963**: 163699. (LA-UR-19-28775 DOI: 10.1016/j.nima.2020.163699)

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Reports

DiGiovine, B. J. WNR Facility T4GEN2 Spallation Target Upgrade. Unpublished report. (LA-UR-20-30500)

DiGiovine, B. J. and L. Zavorka. WNR Facility Flight Path 90L Advanced Collimation Development. Unpublished report. (LA-UR-21-20779)

Lee, H. Y. Pinning Down the nu-p Process Importance in Heavy Element Production via Reaction Studies on Radioactive 56Ni at LANSCE. Unpublished report. (LA-UR-17-30772)

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Grinder, M. M. and H. Y. Lee. Diamond Detectors in High Radiation Background. Presented at *NSSC-LANL Keepin Program presentation*, Los Alamos, New Mexico, United States, 2018-08-08 - 2018-08-08. (LA-UR-18-27519)

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Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, A. Georgiadou, L. Zavorka and H. I. Kim. Measurement of 35Cl(n,p)35S at LANSCE. Presented at *CSEWG*, Brookhaven, New York, United States, 2019-11-04 - 2019-11-06. (LA-UR-19-31100)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, S. M. Mosby, F. M. Nortier, C. Vermeulen, P. Tsintari, G. Perdikakis and M. M. Grinder. Constraining the \xce\xbdp-process through the study of neutron-induced charged-particle reactions on short-lived 56Ni. Presented at *APS April Meeting*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23602)

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Lee, H. Y., B. J. DiGiovine, L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, E. R. Birnbaum, M. Brugh, S. A. Kozimor, V. Mocko, F. M. Nortier, H. I. Kim, G. Perdikakis, P. Tsintari, C. Frohlich and M. Grinder. LENZ at LANSCE: neutron-induced charged-particle reaction studies on radioactive nuclei. Presented at *CENTAUR Scientific Advisory Committee Meeting*, Los Alamos, New Mexico, United States, 2019-08-21 - 2019-08-23. (LA-UR-19-28495)

Lee, H. Y., B. J. DiGiovine, L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, E. R. Birnbaum, M. Brugh, S. A. Kozimor and V. Mocko. LENZ at LANSCE: neutron-induced charged-particle reaction studies on radioactive nuclei. Presented at *Nuclear Data Workshop*, Livermore, California, United States, 2019-09-09 - 2019-09-13. (LA-UR-19-28969)

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Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, D. G. J. Votaw, L. Zavorka, C. Vermeulen, C. Eiroa Lledo, V. Mocko, E. R. Birnbaum, G. Perdikakis, P. Tsintari, C. Frohlich and T. Kawano. Direct measurement on radioactive 56,59Ni(n,p) reactions at Los Alamos Neutron Science Center (LANSCE). Presented at *The Institute of Nuclear and Particle Physics Seminar at Ohio University*, Athens, Ohio, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-29835)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, D. G. J. Votaw, L. Zavorka, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, V. Mocko, E. R. Birnbaum, G. Perdikakis, P. Tsintari and C. Frohlich. Direct measurement of neutron-induced reactions with radioactive 56,59Ni at Los Alamos Neutron Science Center (LANSCE). Presented at *2021 SSAP Symposium Stewardship Science Academic Programs Annual Review*, washington DC, District Of Columbia, United States, 2021-02-16 - 2021-02-18. (LA-UR-21-21448)

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Vermeulen, C., H. Y. Lee, E. R. Birnbaum, F. M. Nortier, S. A. Kuvin, K. Bennett and G. Pederkakis. Radioactive Targets at Los Alamos National Laboratory: A quasi-philosophical approach. Presented at *25th Conference on Application of Accelerators in Research and Industry*, Grapevine, Texas, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27361)

Posters

Grinder, M., H. Iwasaki, T. Mijatovic, R. Elder, J. Ash, A. Revel, H. Y. Lee and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Implementation of a Radiation-hard Diamond Active Target. Presented at *NSSC University Program Review 2019*, Releigh, North Carolina, United States, 2019-06-04 - 2019-06-06. (LA-UR-19-24418)

Grinder, M., H. Iwasaki, T. Mijatovic, R. Elder, J. Ash, H. Y. Lee and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Diamond Detectors in High Radiation Background. Presented at *The Nuclear Science and Security*

Consortium Fall Workshop, Livermore, California, United States, 2018-10-01 - 2018-10-02. (LA-UR-18-29099)

Grinder, M., H. Y. Lee, H. Iwasaki, T. Mijatovic, R. Elder, J. Ash and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Implementation of a Radiation-Hard Active Target. Presented at *NSSC University Program Review 2018*, Ann Arbor, Michigan, United States, 2018-06-05 - 2018-06-07. (LA-UR-18-23629)

Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, C. Vermeulen and C. Eiroa Lledo. Measurement of the\xc2\xa059Ni(n,p) reaction at LANSCE and progress towards the first direct measurement of the 56Ni(n,p) reaction. Presented at *agnew showcase*, los alamos, New Mexico, United States, 2019-12-10 - 2019-12-10. (LA-UR-19-32221)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, M. Grinder, S. M. Mosby, F. M. Nortier, G. Perdikakis, P. Tsintari and C. Vermeulen. Constraining the nu p-process through the study of neutron-induced charged-particle reactions on short-lived 56Ni. Presented at *Conference on Compound Nuclear Reactions*, Berkeley, California, United States, 2018-09-24 - 2018-09-28. (LA-UR-18-29018)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, M. Grinder, S. M. Mosby, F. M. Nortier, G. Perdikakis, P. Tsintari and C. Vermeulen. First Direct Measurement of the 56Ni(n,p) Reaction. Presented at *LANSCE User Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-07. (LA-UR-18-30461)

Kuvin, S. A. and L. Collaboration. Progress towards the first direct measurement of the 56Ni(n,p) reaction. Presented at *Gordon Research Conference*, New London, New Hampshire, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25358)

Tsintari, P., G. Perdikakis, J. Davison, Z. Purcell, H. Y. Lee, L. Zavorka and C. Frohlich. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *WE-Heraeus summer school on Nuclear Physics in Astrophysics*, Heidelberg, Germany, 2019-09-10 - 2019-09-14. (LA-UR-19-29021)

Tsintari, P., G. Perdikakis, J. Davison, Z. Purcell and H. Y. Lee. Optimization of the LENZ detector system at LANL for the study of (n,p) reactions with radioactive targets using GEANT4 simulations. . (LA-UR-18-29098)

Ultra-Diffuse Galaxies, Tidal Streams and Dwarf Galaxies: The Low-Surface Brightness Frontier

W Vestrand
20180257ER

Project Description

Detecting low surface brightness features is a long standing challenge for optical imagers that are conducting national security missions. The new imaging technology and image software that we are developing will dramatically improve the ability to detect low surface brightness features that would otherwise has gone undetected. Successful development of technology has the potential to favorably impact our capability to conduct the DOE/NNSA treaty monitoring mission. Additionally, it is likely to have important application to difficult remote sensing problems like the detection of plumes and chemical release clouds.

Publications

Journal Articles

*Bellm, E. C., S. R. Kulkarni, M. J. Graham, R. Dekany, R. M. Smith, R. Riddle, F. J. Masci, G. Helou, T. A. Prince, S. M. Adams, C. Barbarino, T. Barlow, J. Bauer, R. Beck, J. Belicki, R. Biswas, N. Blagorodnova, D. Bodewits, B. Bolin, V. Brinnel, T. Brooke, B. Bue, M. Bulla, R. Burruss, S. B. Cenko, C. Chang, A. Connolly, M. Coughlin, J. Cromer, V. Cunningham, K. De, A. Delacroix, V. Desai, D. A. Duev, G. Eadie, T. L. Farnham, M. Feeney, U. Feindt, D. Flynn, A. Franckowiak, S. Frederick, C. Fremling, A. Gal-Yam, S. Gezari, M. Giomi, D. A. Goldstein, V. Z. Golkhou, A. Goobar, S. Groom, E. Hacopians, D. Hale, J. Henning, A. Y. Q. Ho, D. Hover, J. Howell, T. Hung, D. Huppenkothen, D. Imel, W. Ip, Z. Ivezic, E. Jackson, L. Jones, M. Juric, M. M. Kasliwal, S. Kaspi, S. Kaye, M. S. P. Kelley, M. Kowalski, E. Kramer, T. Kupfer, W. Landry, R. R. Laher, C. Lee, H. W. Lin, Z. Lin, R. Lunnan, M. Giomi, A. Mahabal, P. Mao, A. A. Miller, S. Monkewitz, P. Murphy, C. Ngeow, J. Nordin, P. Nugent, E. Ofek, M. T. Patterson, B. Penprase, M. Porter, L. Rauch, U. Rebbapragada, D. Reiley, M. Rigault, H. Rodriguez, J. van Roestel, B. Rusholme, J. van Santen, S. Schulze, D. L. Shupe, L. P. Singer, M. T. Soumagnac, R. Stein, J. Surace, J. Sollerman, P. Szkody, F. Taddia, S. Terek, A. Van Sistine, S. van Velzen, W. T. Vestrand, R. Walters, C. Ward, Q. Ye, P. Yu, L. Yan and J. Zolkower. The Zwicky Transient Facility: System Overview, Performance, and First Results. 2019. *Publications of the Astronomical Society of the Pacific*. **131** (995): 018002. (LA-UR-19-22558 DOI: 10.1088/1538-3873/aaecbe)

*Graham, M. J., S. R. Kulkarni, E. C. Bellm, S. M. Adams, C. Barbarino, N. Blagorodnova, D. Bodewits, B. Bolin, P. R. Brady, S. B. Cenko, C. Chang, M. W. Coughlin, K. De, G. Eadie, T. L. Farnham, U. Feindt, A. Franckowiak, C. Fremling, S. Gezari, S. Ghosh, D. A. Goldstein, V. Z. Golkhou, A. Goobar, A. Y. Q. Ho, D. Huppenkothen, Z. Ivezic, R. L. Jones, M. Juric, D. L. Kaplan, M. M. Kasliwal, M. S. P. Kelley, T. Kupfer, C. Lee, H. W. Lin, R. Lunnan, A. A. Mahabal, A. A. Miller, C. Ngeow, P. Nugent, E. O. Ofek, T. A. Prince, L. Rauch, J. van Roestel, S. Schulze, L. P. Singer, J. Sollerman, F. Taddia, L. Yan, Q. Ye, P. Yu, T. Barlow, J. Bauer, R. Beck, J. Belicki, R. Biswas, V. Brinnel, T. Brooke, B. Bue, M. Bulla, R. Burruss, A. Connolly, J. Cromer, V. Cunningham, R. Dekany, A. Delacroix, V. Desai, D. A. Duev, M. Feeney, D. Flynn, S. Frederick, A. Gal-Yam, M. Giomi, S. Groom, E. Hacopians, D. Hale, G. Helou, J. Henning, D. Hover, L. A. Hillenbrand, J. Howell, T. Hung, D. Imel, W. Ip, E. Jackson, S. Kaspi, S. Kaye, M. Kowalski, E. Kramer, M. Kuhn, W. Landry, R. R. Laher, P. Mao, F. J. Masci, S. Monkewitz, P. Murphy, J. Nordin, M. T. Patterson, B. Penprase, M. Porter, U. Rebbapragada, D. Reiley, R. Riddle, M. Rigault, H. Rodriguez, B. Rusholme, J. van Santen, D. L. Shupe, R. M. Smith, M. T. Soumagnac, R. Stein, J. Surace, P. Szkody, S. Terek, A. Van Sistine, S. van Velzen, W. T. Vestrand, R. Walters, C. Ward, C. Zhang and J. Zolkower. The Zwicky Transient Facility: Science Objectives. 2019. *Publications of the Astronomical Society of the Pacific*. **131** (1001): 078001. (LA-UR-19-30653 DOI: 10.1088/1538-3873/ab006c)

*Panaitescu, A. X-Ray Afterglows from the Gamma-Ray Burst "Large-angle" Emission. 2020. *The Astrophysical Journal*. **895** (1): 39. (LA-UR-20-21724 DOI: 10.3847/1538-4357/ab8bdf)

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Vestrand, W. T. and L. P. Parker. Optical Emission from Fossil Cosmic Ray Reservoirs. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-27021)

Conference Papers

Parker, L. P., Y. H. Sechrest, W. T. Vestrand, P. R. Wozniak and D. Palmer. A Heterogeneous Telescope Array Optimized For Low Surface Brightness Imaging. Presented at *SPIE Astronomical Telescopes + Instrumentation (digital, remote)*. (Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16). (LA-UR-20-29825)

Presentation Slides

Parker, L. P. A Heterogeneous Telescope Array Optimized For Low Surface Brightness Imaging. Presented at *SPIE Astonomical Telescopes + Instrumentation (digital, remote)*, Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-29819)

Posters

Parker, L. P. A Heterogeneous Telescope Array Optimized For Low Surface Brightness Imaging. Presented at *SPIE Astronomical Telescopes + Instrumentation (digital, remote conference)*, Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-29826)

Using Quarkonia to Probe Matter from the Early Universe

Ivan Vitev
20190033ER

Project Description

A millionth of a second after the Big Bang, while still at a temperature of several trillion degrees, the entire universe transitioned through a phase of matter we are only beginning to understand--- the quark-gluon plasma (QGP), a hot and dense soup of the most fundamental microscopic constituents that make up the visible world. As this strongly interacting plasma expanded and cooled down, quarks and gluons clumped together into bound states to form a gas of particles called hadrons. This phase transition is of great interest to particle and nuclear physics, cosmology and astrophysics. It was predicted to affect the density of dark matter, and result in gravitational waves that probe the QGP properties. Heavy ion physics is a forefront area of research at the interface of high-energy and nuclear science that seeks to recreate these primordial states of matter of the early universe in controlled laboratory conditions and pin down their properties by colliding nuclei at ultrarelativistic energies. We will develop a new theory that describes some of the heaviest elementary particles produced in nature, called quarkonia, and use them to determine the properties of a primordial state of matter created in heavy ion collisions and the early universe.

Publications

Journal Articles

Fleming, S., Y. Makris and T. Mehen. An effective field theory approach to quarkonium at small transverse momentum. Submitted to *Journal of High Energy Physics*. (LA-UR-19-31110)

*Gao, A., H. T. Li, I. Moult and H. X. Zhu. Precision QCD Event Shapes at Hadron Colliders: The Transverse Energy-Energy Correlator in the Back-to-Back Limit. 2019. *Physical Review Letters*. **123** (6): 062001. (LA-UR-19-20914 DOI: 10.1103/PhysRevLett.123.062001)

Gutierrez-Reyes, D., Y. Makris, V. P. Vaidya, I. Scimemi and L. Zoppi. Probing Transverse-Momentum Distributions With Groomed Jets. Submitted to *Journal of High Energy Physics*. (LA-UR-19-31102)

*Kang, Z., J. Reiten, I. Vitev and B. Yoon. Light and heavy flavor dijet production and dijet mass modification in heavy ion collisions. 2019. *Physical Review D*. **99** (3): 034006. (LA-UR-19-22344 DOI: 10.1103/PhysRevD.99.034006)

*Lee, C., P. Shrivastava and V. Vaidya. Predictions for energy correlators probing substructure of groomed heavy quark jets. 2019. *Journal of High Energy Physics*. **2019** (9): 45. (LA-UR-18-24853 DOI: 10.1007/JHEP09(2019)045)

*Li, C. S., H. T. Li, D. Y. Shao and J. Wang. Momentum-space threshold resummation in tW production at the LHC. 2019. *Journal of High Energy Physics*. **2019** (6): 125. (LA-UR-19-21475 DOI: 10.1007/JHEP06(2019)125)

Li, H. T. and I. Vitev. Jet splitting function in the vacuum and QCD medium. *PoS - Proceedings of Science*. (LA-UR-19-20679 DOI: 10.22323/1.345.0077)

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Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in h \xe2\x86\x92\xce\xb3\xce\xb3 Decay: II. Renormalization and Scale Evolution. Submitted to *Journal of High Energy Physics*. (LA-UR-20-28938)

Makris, Y. Mitigating large background using subtracted jet substructure moments. Submitted to *Physical Review D*. (LA-UR-18-31092)

Makris, Y. and I. M. Vitev. An Effective Theory of Quarkonia in QCD Matter. Submitted to *Journal of High Energy Physics*. (LA-UR-19-25833)

*Sievert, M. D., I. Vitev and B. Yoon. A complete set of in-medium splitting functions to any order in opacity. 2019. *Physics Letters B*. **795**: 502-510. (LA-UR-19-22343 DOI: 10.1016/j.physletb.2019.06.019)

Vitev, I. Aspects of heavy flavor jet physics in heavy ion collisions. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30718 DOI: 10.22323/1.355.0009)

Vitev, I. Toward an effective theory of quarkonium production nuclear matter. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30716 DOI: 10.22323/1.355.0041)

Vitev, I. M., A. Sadofyev and M. Sievert. Ab Initio Coupling of Jets to Collective Flow in the Opacity Expansion Approach. Submitted to *Journal of High Energy Physics*. (LA-UR-21-21420)

Vitev, I. M., H. Li and Z. Liu. Heavy meson tomography of cold nuclear matter at the electron-ion collider. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-20-28004)

Vitev, I. M. and J. Lansberg. Perspectives for quarkonium studies at high-luminosity LHC. Submitted to *Elsevier journal family*. (LA-UR-20-28018)

Vitev, I. M. and Y. Makris. An Effective Theory of Quarkonia in QCD Matter. Submitted to *Nuclear Physics A*. (LA-UR-20-28019)

Books/Chapters

Lee, C., I. M. Vitev, R. Boussarie, J. W. Qiu, I. W. Stewart, T. Mehen, M. Burkardt, M. Constantinou, W. Detmold, M. Ebert, M. Engelhardt, S. Fleming, L. Gamberg, X. Ji, Z. B. Kang, K. F. Liu, S. Liuti, A. Metz, J. Negele, D. Pitonyak, A. Prokudin, A. Rajan, M. Schlegel, P. Shanahan, P. Schweitzer, A. Tarasov, R. Venugopalan, F. Yuan and Y. Zhao. TMD Handbook: A modern introduction to the physics of Transverse Momentum Dependent distributions. (LA-UR-21-20798)

Da Silva, C. L., J. M. Durham, C. Lee, X. Li, M. X. Liu, A. Morreale, W. E. Sondheim, I. M. Vitev, B. Surrow, R. Milner, A. Dumitru, O. Evdomikov, A. Metz, C. Mu\xc3\xb1oz Camacho, K. Barish, T. Horn, P. Jones, S. Dalla Torre, M. Diefenthaler and C. Wong. EIC Yellow Report. (LA-UR-21-20953)

Reports

Vitev, I. M. Future physics opportunities for high-density QCD at the LHC with heavy-ion and proton beam. Unpublished report. (LA-UR-19-22345)

Ultra-Cold Neutron Experiment for Proton Branching Ratio in Neutron Beta Decay (UCNProBe)

Zhaowen Tang
20190048ER

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.

Publications

Journal Articles

Tang, Z., E. B. Watkins, S. Clayton, S. A. Currie, D. E. Fellers, M. T. Hassan, D. E. Hooks, T. Ito, S. K. Lawrence, S. W. T. MacDonald, M. F. Makela, C. Morris, L. P. Neukirch, A. Saunders, C. M. O'Shaughnessy, C. B. Cude-Woods, J. H. Choi, A. R. Young, B. A. Zeck, F. M. Gonzalez, C. Liu, N. C. Floyd, K. P. Hickerson, B. A. Johnson, J. C. Lambert, R. W. J. Pattie and A. T. Holley. Ultracold Neutron Properties of the Eljen-299-02D deuterated scintillator. Submitted to *Review of Scientific Instruments*. (LA-UR-20-27508)

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)

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., 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)

Wideband Sub-Millimeter Source for Deployed Applications

Kip Bishofberger
20190066ER

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).

Publications

Journal Articles

Yampolsky, N. and K. A. Bishofberger. Description of longitudinal space charge effects in beams and plasma through dielectric permittivity. Submitted to *Physical Review Applied*. (LA-UR-21-21464)

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)

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)

Ultralight Bosonic Dark Matter Search with an Optically Pumped Magnetometer

Leanne Duffy
20190113ER

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.

Publications

Reports

Milton, S. V. Review of LDRD ER Project 20190113ER. Unpublished report. (LA-UR-21-20385)

Presentation Slides

Duffy, L. D. Axion search with the Axion Dark Matter eXperiment and other new idea(s). . (LA-UR-20-28374)

Kim, Y. J., P. Chu, I. M. Savukov, S. G. Newman, L. D. Duffy and A. V. Urbaitis. Dark Matter and Fundamental Physics Searches using Atomic Magnetometers. Presented at *CPAD Instrumentation Frontier Workshop 2019*, Madison, Wisconsin, United States, 2019-12-08 - 2019-12-10. (LA-UR-19-31996)

Hot Electron Beam Generation and Transport for Fast Ignition

Sasikumar Palaniyappan
20190124ER

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.

Publications

Journal Articles

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)

Presentation Slides

Huang, C., F. Li, P. K. Singh and S. Palaniyappan. Transport of low-divergence high-current electron beams in a high density plasma. Presented at *49th Annual Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-10 - 2019-06-14. (LA-UR-19-25186)

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)

A New Computation Framework for the Nonlinear Beam Dynamics with Radiation Self-fields

Chengkun Huang
20190131ER

Project Description

The development of X-ray Free Electron Lasers (FELs) and compact advanced accelerators provides the foundation to address the control of performance and production of materials at the mesoscale, a major challenge in national security missions. The continuing quest to enhance the performance/functionality of X-ray FELs and advance accelerators demands techniques to manipulate electron beams with the highest brightness. However, nonlinear beam dynamic problems often arise in the generation and control of such beams. State-of-the-art theoretical and simulation models lack the accuracy and physics consistency to fully address these outstanding beam dynamic problems. We will design and implement a new simulation framework to treat the self-consistent dynamics of a relativistic particle beam interacting with its complete radiation self-fields. With the unprecedented accuracy and physics consistency, this tool will be applied to the evaluation of high risk component design in free electron lasers.

Publications

Conference Papers

Li, F., C. Huang, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Validation of a novel method for the calculation of near-field synchrotron radiation. Presented at *10th International Particle Accelerator Conference*. (Melbourne, Australia, 2019-05-19 - 2019-05-24). (LA-UR-19-24377)

Reports

Gress, G. J. Understanding machine learning approaches for partial differential equations. Unpublished report. (LA-UR-20-27592)

Yeung, O. B. Validation of Two-Dimensional Near-Field Synchrotron Radiation Solver. Unpublished report. (LA-UR-19-27333)

Presentation Slides

Huang, C. Particle accelerators: present, future and the enabling computational modeling. . (LA-UR-19-31915)

Huang, C., F. Li, H. N. Rakotoarivelo, B. Shen, R. V. Garimella, O. B. Yeung, P. P. Pombrio, T. J. T. Kwan and B. E. Carlsten. A Particle-Mesh Method for the Modeling of Synchrotron Radiation from Electron Beam. Presented at *47th IEEE International Conference On Plasma Sciences (virtual)*, online, New Mexico, United States, 2020-12-06 - 2020-12-10. (LA-UR-20-29999)

Huang, C., F. Li, H. N. Rakotoarivelo, O. B. Yeung, P. P. Pombrio, B. Shen, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. A Particle-Mesh Method for the Modeling of Synchrotron Radiation from Electron Beam. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, online, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29142)

Huang, C., F. Li, O. B. Yeung, P. P. Pombrio, B. Shen, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Comparison of Numerical Methods for the Calculation of Synchrotron Radiation from Electrons. 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-19-30731)

Li, F., C. Huang, O. B. Yeung, B. Shen, P. P. Pombrio, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Comparison of Numerical Methods for the Calculation of Synchrotron Radiation from Electrons. Presented at *North American Particle Accelerator Conference*, Lansing, Michigan, United States, 2019-09-01 - 2019-09-06. (LA-UR-19-28858)

Shen, B. Numerical Method and Parallelization for the Computation of Synchrotron Radiation. Presented at *Super Computing 2019*, Denver, Colorado, United States, 2019-11-17 - 2019-11-17. (LA-UR-19-27982)

Yeung, O. B. Design and Validation of a Solver for Synchrotron Radiation. Presented at *LANL SULI Presentations, on-site*, Los Alamos, New Mexico, United States, 2019-07-17 - 2019-07-17. (LA-UR-19-27178)

Posters

Li, F., C. Huang, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Validation of a novel method for the calculation of near-field synchrotron radiation. Presented at *10th International Particle Accelerator Conference*, Melbourne, Australia, 2019-05-19 - 2019-05-24. (LA-UR-19-24589)

Shen, B. Numerical Method and Parallelization for the Computation of Synchrotron Radiation. Presented at *Super Computing 19*, Denver, Colorado, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-27461)

Shen, B. Numerical Method for the Computation of Synchrotron Radiation in the Near-Field. Presented at *PCSRI Outbrief Presentations*, Los alamos, New Mexico, United States, 2019-07-30 - 2019-07-30. (LA-UR-19-27494)

The Influence of Multiple Scattering on the Opacities of Warm and Hot Dense Matter

Charles Starrett
20190206ER

Project Description

Opacity is a key quantity in weapons physics as well as inertial fusion and astrophysics. Our project will develop an new computational capability for opacity in dense plasmas -- a significant improvement over existing methods. The key advantage of our approach is that plasma effects will be fully accounted for in a non-perturbative way, in contrast to existing methods. We will apply this to open and enigmatic experiments that point to weaknesses in current approaches.

Publications

Journal Articles

Gill, N. M., C. E. Starrett and C. J. Fontes. Time-Dependent Density Functional Theory Applied to Average Atom Opacity. Submitted to *Physical Review E*. (LA-UR-21-20133)

Starrett, C. E. and N. R. Shaffer. Multiple Scattering Theory for Dense Plasmas. Submitted to *Physical Review E*. (LA-UR-20-26583)

White, J. R., W. R. Johns, C. J. Fontes, N. M. Gill, N. R. Shaffer and C. E. Starrett. Charge State Distributions in Dense Plasmas. Submitted to *High Energy Density Physics*. (LA-UR-20-27503)

Reports

Abrams, J. R., B. W. Bell, T. S. Blade, J. W. Dyer, F. Holguin, J. S. Keithley, H. Leiendecker, W. R. Johns, E. C. Koskelo, N. Y. Lo, O. G. Martin, A. P. May, T. M. Natan, L. V. Nguyen, C. F. Ottoway, D. A. Owens, S. D. Ozier, A. D. Somers, T. J. Taylor, A. J. Warhover, J. R. White, Q. M. White, C. J. Young, M. T. Andrews, G. R. Maskaly and D. M. Israel. Final Reports of the 2020 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-20-28407)

Alberse, J. R., A. E. Biewer, S. E. Campbell, H. S. Chalfin, C. A. J. Coffelt, D. K. Coffman, B. H. Fore, J. A. Freiberg, C. J. Hanson, S. Hegde, B. F. Hellwig, S. Joshi, C. R. Kumar, M. W. Laraia, J. T. Laune, L. L. Lin, C. X. Meng, A. M. Nemeth, C. S. Parker, D. M. Perez, S. Pineda, T. A. Saxton, T. Skaras, M. T. Andrews, D. M. Israel and G. R. Maskaly. Final Reports of the 2019 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-21-21581)

Gill, N. M. Modeling of Warm Dense Plasmas for the Determination of Transport Properties and Equation of State. Unpublished report. (LA-UR-20-22190)

Laraia, M. W., C. J. Hanson, N. R. Shaffer, D. Saumon, D. P. Kilcrease and C. E. Starrett. Real-Space Green's functions for Warm Dense Matter. Unpublished report. (LA-UR-20-30465)

Presentation Slides

Shaffer, N. R. and C. E. Starrett. Dense Plasma Opacity via Multiple Scattering Theory. Presented at *HED theory group meeting*, Rochester, New York, United States, 2021-03-11 - 2021-03-11. (LA-UR-21-22320)

Starrett, C. E. Electronic structure of Dense Plasma’s with the Green’s Function Method. . (LA-UR-19-29084)

Starrett, C. E. Towards a Complete and Consistent Model for Material Properties at Extreme Conditions. Presented at *NNSA ICF working group*, Remote, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-30249)

Starrett, C. E. and N. R. Shaffer. Multiple Scattering Theory for Dense Plasma Electronic Structure. . (LA-UR-20-27878)

Starrett, C. E. and N. R. Shaffer. Multiple Scattering Theory for Dense Plasma Electronic Structure. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22323)

White, J. R., W. R. Johns, C. E. Starrett, N. R. Shaffer, C. J. Fontes and N. M. Gill. Photon Transport in Warm Dense Matter. . (LA-UR-20-26113)

Posters

Hanson, C. J., M. W. Laraia, C. E. Starrett, N. R. Shaffer and D. P. Kilcrease. Microfield distributions from pseudoatom molecular dynamics & Real-space structures for multiple scattering green’s functions. . (LA-UR-19-27904)

Starrett, C. E. Using the Green’s Function Multiple Scattering Method to Model Warm and Hot Dense Matter. Presented

at *2019 Workshop on Recent Developments in Electronic Structure*, Urbana, Illinois, United States, 2019-05-19 - 2019-05-19. (LA-UR-19-24197)

A Non-Invasive Current Profile Diagnostic for Electron Bunches

Quinn Marksteiner
20190294ER

Project Description

This project will develop an electron beam diagnostic that will help resolve many important physics issues for high energy electron accelerators. This diagnostic will be of particular importance for accelerator capabilities, where a non-invasive diagnostic with short (femtosecond) resolution is needed to address important issues such as the microbunching instability and long-range wakes. In addition, the Department of Energy Office of Science Advanced Accelerator Development Strategy Report specifically calls out the need for diagnostics with femtosecond resolution, for laser-driven plasma wakefield accelerators and for particle-beam-driven plasma wakefield accelerators.

Publications

Journal Articles

*Yampolsky, N., E. I. Simakov and A. Malyzhenkov. Imposing strong correlated energy spread on relativistic bunches with transverse deflecting cavities. 2020. *Physical Review Accelerators and Beams*. **23** (5): 054403. (LA-UR-19-30405 DOI: 10.1103/PhysRevAccelBeams.23.054403)

Presentation Slides

Marksteiner, Q. R., H. L. Andrews, S. Barber, J. E. Coleman, C. Emma, B. W. Ostler, W. P. Romero, R. Ryne and N. Yampolsky. Using off axis undulator radiation as a longitudinal current diagnostic. Presented at *Advanced Control Methods for Particle Accelerators*, Santa Fe, New Mexico, United States, 2019-08-20 - 2019-08-22. (LA-UR-19-28705)

Ostler, B. W. Developing a single-shot, nondestructive, and femtosecond resolution longitudinal charge density diagnostic for electron bunches; script. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25782)

Ostler, B. W., Q. R. Marksteiner, N. Yampolsky, H. L. Andrews, S. Barber, J. E. Coleman, C. Emma, W. P. Romero, R. D. Ryne, M. R. A. Zuboraj and J. van Tilborg. A High-Resolution and Noninvasive Longitudinal Profile Diagnostic for Electron Bunches. Presented at *Advanced Accelerator Concepts Seminar Series 2020 (Virtual)*, Los Alamos, New Mexico, United States, 2020-11-18 - 2021-02-03. (LA-UR-21-20100)

Ostler, B. W., Q. R. Marksteiner, N. Yampolsky, R. D. Ryne, R. L. Fleming, S. Barber, C. Emma and W. P. Romero. Developing a single-shot, nondestructive, and femtosecond resolution longitudinal charge density diagnostic for electron bunches. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25684)

Origin of High-Energy Astrophysical Neutrinos: Multi-messenger Signals from Flares of Extragalactic Jets

Hui Li
20190383ER

Project Description

This project aims at understanding the origin of high-energy astrophysical neutrinos, especially those made by relativistic jets powered by supermassive black holes. This is a fundamental question in our understanding of the cosmos. This project brings together theory, numerical modeling, observations in optical and 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.

Publications

Journal Articles

*Abeysekara, A. U., A. Albert, R. Alfaro, C. Alvarez, J. D. Alvarez, J. R. Angeles Camacho, R. Arceo, J. C. Arteaga-Velazquez, K. P. Arunbabu, D. Avila Rojas, H. A. A. Solares, V. Baghmanyan, E. Belmont-Moreno, S. Y. BenZvi, C. Brisbois, K. S. Caballero-Mora, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. Coutino de Leon, E. De la Fuente, C. de Leon, S. Dichiara, B. L. Dingus, M. A. DuVernois, J. C. Diaz-Velez, R. W. Ellsworth, K. Engel, C. Espinoza, B. Fick, H. Fleischhack, N. Fraija, A. Galvan-Gamez, J. A. Garcia-Gonzalez, F. Garfias, M. M. Gonzalez, J. A. Goodman, J. P. Harding, S. Hernandez, J. Hinton, B. Hona, F. Hueyotl-Zahuantitla, C. M. Hui, P. Huntemeyer, A. Iriarte, A. Jardin-Blicq, V. Joshi, S. Kaufmann, D. Kieda, A. Lara, W. H. Lee, H. Leon Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, J. Lundeen, K. Malone, S. S. Marinelli, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, H. Martinez-Huerta, 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, A. Peisker, E. G. Perez-Perez, J. Pretz, Z. Ren, C. D. Rho, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, E. Ruiz-Velasco, H. Salazar, F. S. Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, M. S. Arroyo, G. Sinnis, A. J. Smith, R. W. Springer, P. Surajbali, E. Tabachnick, M. Tanner, O. Tibolla, K. Tollefson, I. Torres, T. Weisgarber, S. Westerhoff, J. Wood, T. Yapici, A. Zepeda and H. Zhou. Measurement of the Crab Nebula Spectrum Past 100 TeV with HAWC. 2019. *The Astrophysical Journal*. **881** (2): 134. (LA-UR-19-24703 DOI: 10.3847/1538-4357/ab2f7d)

*Albert, A., R. Alfaro, D. Avila Rojas, V. Baghmanyan, E. Belmont-Moreno, C. Brisbois, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. Coutino de Leon, E. De la Fuente, C. de Leon, S. Dichiara, K. Engel, C. Espinoza, H. Fleischhack, N. Fraija, A. Galvan-Gamez, D. Garcia, F. Garfias, S. Hernandez, J. Hinton, B. Hona, D. Huang, F. Hueyotl-Zahuantitla, P. Huntemeyer, A. Iriarte, A. Jardin-Blicq, V. Joshi, S. Kaufmann, D. Kieda, A. Lara, H. Leon Vargas, G. Luis-Raya, J. Lundeen, R. Lopez-Coto, K. Malone, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, H. Martinez-Huerta, P. Miranda-Romagnoli, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, R. Noriega-Papaqui, A. Peisker, J. Pretz, Z. Ren, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, E. Ruiz-Velasco, F. S. Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, G. Sinnis, P. Surajbali, E. Tabachnick, M. Tanner, O. Tibolla, K. Tollefson, I. Torres, R. Torres-Escobedo, L. Villasenor, T. Weisgarber, J. Wood, T. Yapici, H. Zhang, H. Zhou, B. L. Dingus and J. P. Harding. Multiple Galactic Sources with Emission Above 56 TeV Detected by HAWC. 2020. *Physical Review Letters*. **124** (2): 021102. (LA-UR-19-29232 DOI: 10.1103/PhysRevLett.124.021102)

Chen, Q., K. Nalewajko and B. P. Mishra. Scaling of Magnetic Dissipation and Particle Acceleration in ABC Fields. Submitted to *Journal of Plasma Physics*. (LA-UR-21-20632)

*Fowler, T. K., H. Li and R. Anantua. A Quasi-static Hyper-resistive Model of Ultra-high-energy Cosmic-ray Acceleration by Magnetically Collimated Jets Created by Active Galactic Nuclei. 2019. *The Astrophysical Journal*. **885** (1): 4. (LA-UR-20-28592 DOI: 10.3847/1538-4357/ab44bc)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

*Guo, F., X. Li, W. Daughton, P. Kilian, H. Li, Y. Liu, W. Yan and D. Ma. Determining the Dominant Acceleration Mechanism during Relativistic Magnetic Reconnection in Large-scale Systems. 2019. *Physical Review Letters*. **879** (2). (LA-UR-18-31752 DOI: 10.3847/2041-8213/ab2a15)

Guo, F., X. Li, W. S. Daughton, H. Li, P. F. H. Kilian, Y. H. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics and Particle Acceleration during Relativistic Turbulent Magnetic Reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-26005)

Guo, F., Y. Liu, X. Li, H. Li, W. S. Daughton and P. F. H. Kilian. Recent Progress on Particle Acceleration and Reconnection Physics during Magnetic Reconnection in the Magnetically-dominated Relativistic Regime. Submitted to *Physics of Plasmas*. (LA-UR-20-26135)

Hona, B., S. Casanova, K. Feng, P. Huentemeyer, A. Albert, M. Durocher, J. P. Harding and K. A. Malone. HAWC observations of the acceleration of very-high-energy cosmic rays in the Cygnus Cocoon. Submitted to *Nature Astronomy*. (LA-UR-21-22386)

*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)

*Kong, X., F. Guo, Y. Chen and J. Giacalone. The Acceleration of Energetic Particles at Coronal Shocks and Emergence of a Double Power-law Feature in Particle Energy Spectra. 2019. *Astrophysical Journal*. **883** (1): 49. (LA-UR-19-20913 DOI: 10.3847/1538-4357/ab3848)

*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)

Li, H. Fast Magnetic Reconnection with Turbulence in High Lundquist Number Limit. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-24765)

Li, H. 3D Numerical Simulation of Kink-driven Rayleigh–Taylor Instability Leading to Fast Magnetic Reconnection. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-28588)

Li, H. Energy occupation of waves and structures in 3D compressive MHD turbulence. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-28590)

*Loi, F., M. Murgia, F. Govoni, V. Vacca, A. Bonafede, C. Ferrari, I. Prandoni, L. Feretti, G. Giovannini and H. Li. Rotation measure synthesis applied to synthetic SKA images of galaxy clusters. 2019. *Monthly Notices of the Royal Astronomical Society*. **490** (4): 4841-4857. (LA-UR-20-28593 DOI: 10.1093/mnras/stz2699)

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. 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)

Polko, P. and H. Li. Self-similar jet models: two new issues. Submitted to *Astrophysical Journal*. (LA-UR-19-30944)

Zhang, H., X. Li, D. Giannios, F. Guo, Y. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–I. A Systematic Study. Submitted to *Astrophysical Journal*. (LA-UR-20-20194)

Conference Papers

Dong, B., P. F. H. Kilian, X. Li, F. Guo, S. Byna and K. Wu. Terabyte-scale Particle Data Analysis: An ArrayUDF Case Study. Presented at *SSDBM 2019 : 31st International Conference on Scientific & Statistical Database Management*. (Santa Cruz, California, United States, 2019-07-23 - 2019-07-25). (LA-UR-19-24098)

Malone, K. A. Recent Results from the High Altitude Water Cherenkov Observatory. Presented at *International Symposium on Multiparticle Dynamics*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-13). (LA-UR-20-21318)

Reports

Rani, B., H. Zhang, S. Hunter, F. Kislat, M. Boettcher, J. E. McEnery, D. Giannios, F. Guo, H. Li, M. G. Baring, I. Agudo, S. Buson, M. Petropoulou, V. Pavlidou, E. Angelakis, I. Myserlis, Z. Wadiasingh, R. Curado da Silva, P. F. H. Kilian, S. Guiriec, V. Bozhilov, S. Anton, M. Kazana, P. Coppi, T. M. Venters, F. Longo and E. Bottachini. High-Energy Polarimetry - a new window to probe extreme physics in AGN jets. Unpublished report. (LA-UR-19-22708)

Presentation Slides

Guo, F. IC Project: Magnetic Reconnection versus Shocks: First-principles Kinetic Simulations of Major Particle Acceleration Mechanisms in the Universe. . (LA-UR-19-21782)

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)

H. Kilian, P. F. and F. Guo. Particle Acceleration due to Relativistic Reconnection. Presented at *235th AAS meeting*, Honolulu, Hawaii, United States, 2020-01-05 - 2020-01-08. (LA-UR-20-20084)

Li, H. All Hands On Deck: Understanding Astrophysical Jets. . (LA-UR-19-32437)

Li, H. Origin of High-Energy Astrophysical Neutrinos: Multi-Messenger Signals from Flares of Extra-galactic Jets. . (LA-UR-20-29526)

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)

Atomic Magnetometry for the neutron Electric Dipole Moment (nEDM) Experiment (Rosen Scholar)

Michael Furlanetto

20200003ER

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 significantly contributed to demonstrating a capability to perform next generation experiments looking for neutron electric dipole moment, controlling systematics important for all such experiments. 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 will benefit research performed at the Laboratory and elsewhere.

Effects of Strong Electronic Correlations on the Properties of Warm Dense Matter

Jerome Daligault
20200074ER

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 and in nuclear explosions. 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.

Publications

Journal Articles

Bernstein, D. J., T. Lafleur, J. O. Daligault and S. D. Baalrud. Friction Force in Strongly Magnetized Plasmas. Submitted to *Physical Review E*. (LA-UR-20-25004)

Daligault, J. O., D. J. Bernstein, S. D. Baalrud and T. Lafleur. Friction Force in Strongly Magnetized Plasmas. Submitted to *Physical Review Letters*. (LA-UR-20-23660)

Daligault, J. O., J. Simoni, Q. L. Nguyen, K. M. Dorney, J. L. Ellis, N. J. Brooks, D. D. Hickstein, A. N. Grennell, X. Shi, S. Yazdi, E. E. Campbell, H. C. Kapteyn and M. M. Murnane. Mapping the electron-phonon coupling and hot electron cooling in copper nanoparticles in the warm-dense regime. Submitted to *Nature Physics*. (LA-UR-20-24971)

Daligault, J. O. and J. Simoni. Electronic Friction in Warm Dense Matter. Submitted to *Physical Review Letters*. (LA-UR-20-22846)

Mozyrsky, D. V., E. Stolyarov and A. J. White. Mixed quantum-classical approach to model non-adiabatic electron-nuclear dynamics: Detailed balance and improved surface hopping method. Submitted to *Journal of Chemical Physics*. (LA-UR-20-24033)

Exploration of Neutron-Star Crust Dynamics in the Era of Gravitational-Wave Astrophysics

Irina Sagert
20200145ER

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.

Publications

Journal Articles

Korobkin, O., R. T. Wollaeger, C. L. Fryer, A. L. Hungerford, S. Rosswog, C. J. Fontes, M. R. Mumpower, E. A. Chase, W. P. Even, J. M. Miller, G. W. Misch and J. Lippuner. Axisymmetric Radiative Transfer Models of Kilonovae. Submitted to *Astrophysical Journal*. (LA-UR-20-22607)

Loiseau, J., H. Lim, I. Sagert, M. A. R. Kaltenborn, O. Korobkin, C. M. Mauney, W. P. Even and B. K. Bergen. FleCSPH: The Next Generation FleCSIble Parallel Computational Infrastructure for Smoothed Particle Hydrodynamics. Submitted to *Software X*. (LA-UR-20-23626)

*Murakami, M., O. Korobkin and G. Zhang. Time-dependent density-functional theory of high-order harmonic generation from noble-gas atoms driven by orthogonally polarized two-color laser fields. 2020. *Physical Review A*. **101** (6): 063413. (LA-UR-20-22847 DOI: 10.1103/PhysRevA.101.063413)

Tsao, B., R. Haas and A. Tsokaros. Source term method for binary neutron stars initial data. Submitted to *Journal of Computational Physics*. (LA-UR-20-28227)

Reports

Korobkin, O. Institutional Computing 2019/2020 Project Report: First Year. Unpublished report. (LA-UR-20-25524)

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)

Presentation Slides

Korobkin, O. Mergers of Compact Objects with SPH and General Relativity, Allocation: w20_nsmergers (year 1). . (LA-UR-21-22056)

Lim, H. Are we alone? Searching Intelligent Life Beyond the Earth. . (LA-UR-20-25542)

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. and O. Korobkin. Studying Crust-Breaking Events in Neutron Stars with Strength and Smoothed Particle Hydrodynamics. . (LA-UR-20-21887)

Tews, I. Stringent constraints on neutron-star radii from neutron-star mergers and chiral effective field theory. Presented at *Hirschegg 2020*, Hirschegg, Austria, 2020-01-13 - 2020-01-13. (LA-UR-20-20236)

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)

Other

Lim, H. Are we alone? Searching Intelligent life beyond the Earth. Audio/Visual. (LA-UR-20-27695)

Novel X-ray Free-electron Lasers (XFEL) Accelerator Architecture

Petr Anisimov
20200287ER

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.

Publications

Journal Articles

*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)

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)

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)

MixIT – Understanding Mix in Fusion Implosions through Ion Temperature Imaging

Verena Geppert-Kleinrath
20200324ER

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.

Publications

Presentation Slides

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. and V. Geppert-Kleinrath. MixIT LDRD Lens Design. . (LA-UR-20-24227)

The Missing Link: Quantum Mechanics in Plasma Kinetic Modeling

Mark Zammit
20200356ER

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.

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)

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)

Scarlett, L. H., J. S. Savage, D. V. Fursa, I. Bray, M. C. Zammit and B. I. Schneider. Convergent close-coupling calculations of electrons scattering on electronically-excited molecular hydrogen. Submitted to *Physical Review A*. (LA-UR-20-30414)

Wu\xcc\x88nderlich, D., L. H. Scarlett, S. Briefi, U. Fantz, M. C. Zammit, D. V. Fursa and I. Bray. Application of Molecular Convergent Close-Coupling cross sections in a Collisional Radiative model for the triplet system of molecular hydrogen. Submitted to *Journal of Physics D: Applied Physics*. (LA-UR-20-27482)

Conference Papers

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)

Presentation Slides

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)

Garland, N. A. Impact of a minority relativistic electron tail interacting with a thermal plasma containing high-atomic-number impurities. . (LA-UR-20-23791)

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)

Zammit, M. C., J. A. Leiding, J. C. A. O. Jung, J. P. Colgan, C. J. Fontes, D. P. Kilcrease, P. Hakel, E. M. E. Timmermans, D. V. Fursa and I. Bray. First-Principles Molecular Spectra for Air and Astrophysical Plasmas. Presented at *73rd Annual Gaseous Electronics Virtual Conference*, San Diego, California, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-27919)

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)

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)

How do Pulsar Winds Shine in Tera Electron Volt (TeV)?

Fan Guo
20200367ER

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.

Publications

Journal Articles

Chen, Q., K. Nalewajko and B. P. Mishra. Scaling of Magnetic Dissipation and Particle Acceleration in ABC Fields. Submitted to *Journal of Plasma Physics*. (LA-UR-21-20632)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

Guo, F., X. Li, W. S. Daughton, H. Li, P. F. H. Kilian, Y. H. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics and Particle Acceleration during Relativistic Turbulent Magnetic Reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-26005)

Guo, F., Y. Liu, X. Li, H. Li, W. S. Daughton and P. F. H. Kilian. Recent Progress on Particle Acceleration and Reconnection Physics during Magnetic Reconnection in the Magnetically-dominated Relativistic Regime. Submitted to *Physics of Plasmas*. (LA-UR-20-26135)

Harry, A., J. Drake, M. Swisdak, F. Guo, J. Dahlin, B. Chen, G. Fleishman, L. Glesener, K. Eduard, T. Phan and C. Shen. Electron Acceleration during Macroscale Non-Relativistic Magnetic Reconnection. Submitted to *Physical Review Letters*. (LA-UR-20-30073)

*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)

Kong, X., F. Guo, C. Shen, B. Chen, Y. Chen and J. Giacalone. Dynamical modulation of solar flare electron acceleration due to plasmoid-shock interactions in the looptop region. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-30072)

Li, X., F. Guo and Y. Liu. The Acceleration of Charged Particles and Formation of Power-law Energy Spectra in Nonrelativistic Magnetic Reconnection. Submitted to *Physics of Plasmas*. (LA-UR-21-21365)

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)

Zhang, H., X. Li, D. Giannios, F. Guo, Y. H. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–I. A. Submitted to *Astrophysical Journal*. (LA-UR-20-27998)

zhang, h., X. Li, F. Guo and D. Giannios. First-Principle Prediction of X-ray Polarization from Magnetic Reconnection in High-Frequency BL Lacs. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-30074)

Presentation Slides

Durocher, M. TeV astrophysics with the HAWC observatory. Presented at *APS Four Corners Virtual Meeting*, Albuquerque, New Mexico, United States, 2020-10-23 - 2020-10-24. (LA-UR-20-28463)

Guo, F. Determining the Dominant Acceleration Mechanism during Relativistic Magnetic Reconnection in Large-scale Systems. Presented at *seminar in University of Tokyo.*, Tokyo, Japan, 2020-03-09 - 2020-03-13. (LA-UR-20-20430)

Guo, F. First Principles Kinetic Simulations of Relativistic Collisionless Shocks and Their Particle Acceleration (2019). . (LA-UR-20-25827)

Guo, F. First Principles Kinetic Simulations of Relativistic Collisionless Shocks and Their Particle Acceleration. . (LA-UR-20-25828)

Guo, F. Particle Acceleration in Magnetic Reconnection: From Small Scale to Large Scale. Presented at *2020 Magnetic Reconnection Workshop*, Weihai, China, 2020-08-24 - 2020-08-25. (LA-UR-20-26501)

Harding, J. P. and M. Durocher. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *Virtual APS April Meeting*, Washington, District Of Columbia, United States, 2020-04-18 - 2020-04-18. (LA-UR-20-22988)

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)

H. Kilian, P. F., X. Li, F. Guo and H. Li. Exploring the acceleration mechanisms for particle injection and power-law formation during trans-relativistic magnetic reconnection. Presented at *Understanding the Most Energetic Cosmic Accelerators: Advances in Theory and Simulation*, Online, New Mexico, United States, 2020-10-28 - 2020-10-30. (LA-UR-20-28623)

H. Kilian, P. F. and F. Guo. Particle Acceleration due to Relativistic Reconnection. Presented at *235th AAS meeting*, Honolulu, Hawaii, United States, 2020-01-05 - 2020-01-08. (LA-UR-20-20084)

A Dynamical Approach to Low-Energy Fission

Matthew Mumpower
20200384ER

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.

Publications

Journal Articles

Bulgac, A., I. Abdurrahman, S. Jin, K. Godbey, N. Schunck and I. Stetcu. Fission fragments intrinsic spins and their correlations. Submitted to *Physical Review Letters*. (LA-UR-20-30404)

Verriere, M. and M. R. Mumpower. Improvements to the macroscopic-microscopic approach of nuclear fission. Submitted to *Physical Review C*. (LA-UR-20-26369)

Conference Papers

Mumpower, M. R., M. Verriere and J. Randrup. Macroscopic-microscopic fission yields. Presented at *FUSION20*. (Shizuoka, Japan, 2020-11-15 - 2020-11-15). (LA-UR-20-23186)

Reports

Sprouse, T. M., M. R. Mumpower, I. Stetcu and M. H. Verriere. HPC Requirements Addendum. Unpublished report. (LA-UR-20-26962)

Presentation Slides

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)

Neutrino Physics with Short- and Long-baseline Experiments

Sowjanya Gollapinni
20200539ER

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

*Gollapinni, S., DUNE Collaboration, R. G. Van De Water, W. C. I. Louis, W. E. Sondheim, K. R. Rielage and J. G. Boissevain. Volume III. DUNE far detector technical coordination. 2020. *Journal of Instrumentation*. **15** (08). (LA-UR-20-28752 DOI: 10.1088/1748-0221/15/08/T08009)

*Gollapinni, S., DUNE Collaboration, W. C. I. Louis, R. G. Van De Water, K. R. Rielage, W. E. Sondheim and J. G. Boissevain. Volume I. Introduction to DUNE. 2020. *Journal of Instrumentation*. **15** (08). (LA-UR-20-28748 DOI: 10.1088/1748-0221/15/08/T08008)

*Gollapinni, S., DUNE Collaboration, W. C. I. Louis, R. G. Van De Water, K. R. Rielage, W. E. Sondheim and J. G. Boissevain. Volume IV. The DUNE far detector single-phase technology. 2020. *Journal of Instrumentation*. **15** (08). (LA-UR-20-28763 DOI: 10.1088/1748-0221/15/08/T08010)

Reports

Gollapinni, S., G. Karagiorgi, M. R. Lonegran, W. C. I. Louis, R. G. Van De Water, A. Mogan, G. Yarbrough, W. Tang, MicroBooNE Collaboration and R. Fine. The MicroBooNE Single-Photon Low-Energy Excess Search. Unpublished report. (LA-UR-20-28825)

Gollapinni, S., W. C. I. Louis, R. G. Van De Water, W. E. Sondheim, J. G. Boissevain, K. R. Rielage and DUNE Collaboration. Deep Underground Neutrino Experiment (DUNE), Far Detector Technical Design Report, Volume II: DUNE Physics. Unpublished report. (LA-UR-20-28836)

Presentation Slides

Gollapinni, S. Future Neutrino Experiments and Outlook. Presented at *40th International Conference on High Energy physics - ICHEP2020*, Prague, Czech Republic, 2020-07-28 - 2020-08-06. (LA-UR-21-22366)

Gollapinni, S. Unlocking the Mysteries of Neutrinos with the Deep Underground Neutrino Experiment. . (LA-UR-21-22367)

Gollapinni, S., A. Mogan and MicroBooNE Collaboration. Constraining the Neutral Current Pi0 Background for MicroBooNE's Single-Photon Search. Presented at *Fermilab New Perspective 2.0*, Batavia, Illinois, United States, 2020-08-24 - 2020-08-28. (LA-UR-20-28835)

Gollapinni, S., G. Karagiorgi and MicroBooNE Collaboration. Searches for New Physics with MicroBooNE. Presented at *XXIX International Conference on Neutrino Physics and Astrophysics (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28830)

Gollapinni, S., G. Yarbrough and MicroBooNE Collaboration. Systematic Studies for a Photon-like Low Energy Excess Search at MicroBooNE. Presented at *Fermilab New Perspectives 2.0*, Batavia, Illinois, United States, 2020-08-24 - 2020-08-28. (LA-UR-20-28834)

Gollapinni, S., M. R. Lonegran and MicroBooNE Collaboration. Neutral Current Pi0 Rate Measurement with the MicroBooNE Detector. Presented at *40th International*

Conference on High Energy Physics (ICHEP 2020), Prague, Czech Republic, 2020-07-28 - 2020-08-06. (LA-UR-20-28831)

Posters

Gollapinni, S., A. Mogan and MicroBooNE Collaboration. Constraining the Neutral Current Pi0 Background for MicroBooNE's Single-Photon Search. Presented at *53rd Fermilab Annual Users Meeting*, Batavia, Illinois, United States, 2020-08-10 - 2020-08-14. (LA-UR-20-28832)

Gollapinni, S., G. Yarbrough and MicroBooNE Collaboration. Systematic Studies for a Photon-like Low Energy Excess Search at MicroBooNE. Presented at *53rd Fermilab Annual Users Meeting*, Batavia, Illinois, United States, 2020-08-10 - 2020-08-14. (LA-UR-20-28833)

Gollapinni, S., G. Yarbrough and MicroBooNE Collaboration. Systematic Studies in the Gamma Low Energy Excess Analysis of the MicroBooNE Experiment. Presented at *XXIX INTERNATIONAL CONFERENCE ON NEUTRINO PHYSICS (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28828)

Gollapinni, S., W. Tang and MicroBooNE Collaboration. Detector Systematics Evaluation for the MicroBooNE Single Photon Analysis. Presented at *XXIX INTERNATIONAL CONFERENCE ON NEUTRINO PHYSICS (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28928)

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)

Advanced Fusion Concept for National Security Applications

William Daughton
20200625ER

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 (DOE)/ National Nuclear Security Administration (NNSA). Such experiments would enable researchers to probe the nonlinear physics of thermonuclear burn and to further validate our simulation tools for stockpile stewardship activities.

An Alternative Approach to Inertial Confinement Fusion (ICF) Ignition and Burn Propagation at the National Ignition Facility (NIF)

Richard Olson
20200765ER

Project Description

The National Ignition Facility (NIF) is, by far, the largest laser facility in the world, and our nation has invested billions of dollars in its construction. Additional billions of dollars have been invested, so far, in the unsuccessful indirect drive Inertial Confinement Fusion (ICF) experiments using deuterium–tritium (DT) ice layer implosions. A new innovation to achieve ICF ignition and propagating burn using large Polar Direct Drive (PDD) capsules with liquid DT layers would be an important result for the national laboratories, the National Nuclear Security Administration (NNSA), and the nation. This project builds upon the work of the team responsible for nuclear survivability testing on NIF by not only Los Alamos National Laboratory (LANL), but also Lawrence Livermore National Laboratory (LLNL), Sandia National Laboratories (SNL), the Atomic Weapons Establishment (AWE), the United States Air Force, and the United States Navy. LANL's advanced engineering analysis and system design and analysis groups have been using the existing source for nuclear survivability testing of materials and system components. Achieving ICF ignition would garner world-wide recognition and usher in a new era of weapons-relevant experiments, including needs for studying mix and burn with an ignited plasma in addition to radiation effects testing needs.

Publications

Presentation Slides

Olson, R. E. Concept for increased neutron yield and potential ICF ignition at the NIF. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, on line, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28870)

Nonlinear Dynamics of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams

Lin Yin
20180074ER

Project Description

Achieving inertial fusion ignition in the Laboratory has broad national security implications for understanding the challenging physics inside nuclear weapons. Laser-plasma instabilities (LPI) hamper the ability to compress laser-driven inertial fusion capsules to ignition conditions by decreasing the amount of laser energy that can be used for compression. This project seeks to apply best-in-class modeling capability to understand and mitigate LPI. If successful, the work may enable the design of inertial fusion experiments with higher yield and improved applicability to outstanding weapons science issues.

Technical Outcomes

This project applied large-scale two-dimensional kinetic plasma simulations and analytic theory to understand the complex, nonlinear dynamics of cross beam energy transfer. These innovations enabled the inclusion of effects missing in prior studies, including nonlinear saturation by wave-particle interactions and secondary instabilities involving ion and electron dynamics. A long-term impact of this study is progress toward an improved laser-plasma instabilities (LPI) model suitable for use in the the Advanced Simulation and Computing (ASC) production code, Radiation Adaptive Grid Eulerian (known as "xRAGE" at LANL).

Publications

Journal Articles

*Chen, G., L. Chac\xc3\xb3n, L. Yin, B. J. Albright, D. J. Stark and R. F. Bird. A semi-implicit, energy- and charge-conserving particle-in-cell algorithm for the relativistic Vlasov-Maxwell equations. 2020. *Journal of Computational Physics*. **407**: 109228. (LA-UR-19-21811 DOI: 10.1016/j.jcp.2020.109228)

Stark, D. J., L. Yin, B. J. Albright, A. G. Seaton and R. F. Bird. Stimulated Raman scattering and its interplay with other secondary instabilities in cross-beam-energy-transfer-amplified multi-speckled beams. Submitted to *Physics of Plasmas*. (LA-UR-20-25244)

Yin, L., B. J. Albright, D. J. Stark, R. F. Bird, W. D. Nystrom and K. J. Bowers. Nonlinear electron and ion dynamics in the saturation of crossed-beam energy transfer. Submitted to *Physical Review Letters*. (LA-UR-19-22181)

*Yin, L., B. J. Albright, D. J. Stark, W. D. Nystrom, R. F. Bird and K. J. Bowers. Saturation of cross-beam energy transfer for multispeckled laser beams involving both ion and electron dynamics. 2019. *Physics of Plasmas*. **26** (8): 082708. (LA-UR-19-24839 DOI: 10.1063/1.5111334)

Presentation Slides

Chen, G., L. Chacon, L. Yin, B. J. Albright, D. J. Stark and R. F. Bird. Modern Algorithms for PIC Simulation of Laser-plasma Interactions (LPI). Presented at *SIME Conference ON NONLINEAR WAVES and COHERENT STRUCTURES*, Anaheim, California, United States, 2018-06-11 - 2018-06-14. (LA-UR-18-25421)

Seaton, A. G., L. Yin, R. K. Follett, A. Y. Le and B. J. Albright. Kinetic Modelling of CBET Mitigation Using Laser Bandwidth. Presented at *APS Division of Plasma Physics 2020 Conference*, Virtual, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29049)

Stark, D. J., L. Yin, B. J. Albright, A. G. Seaton and R. F. Bird. Dependence of Cross-Beam Energy Transfer on Plasma Density and Beam Crossing Angle. Presented at *APS DPP Annual Meeting*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-29046)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom and R. F. Bird. Isolating the Role of Ion Trapping in the Saturation of Cross-beam Energy Transfer. Presented at *60th Annual APS DPP meeting*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30538)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom and R. F. Bird. Density dependence of stimulated Raman scattering in CBET-amplified multi-speckle beams. Presented at *Anomalous Absorption*, Telluride, Colorado, United States, 2019-06-10 - 2019-06-10. (LA-UR-19-25205)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom and R. F. Bird. Density dependence of the saturation of stimulated

Raman scattering in CBET-amplified multi-speckled beams. Presented at *61st Annual APS DPP conference*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30512)

Stark, D. J., L. Yin, G. Chen, R. F. Bird, W. D. Nystrom, L. Chacon and B. J. Albright. Nonlinear Dynamics of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams. . (LA-UR-19-21814)

Stark, D. J., L. Yin, K. L. Nguyen, G. Chen, R. F. Bird, W. D. Nystrom, B. J. Albright and L. Chacon. Nonlinear Dynamics of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams. . (LA-UR-20-21983)

Yin, L. Nonlinear electron and ion dynamics in the saturation of cross-beam energy transfer (CBET). Presented at *61st Annual Meeting of the APS-DPP*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30162)

Yin, L., B. J. Albright, D. J. Stark, R. F. Bird and W. D. Nystrom. Nonlinear electron and ion dynamics in the saturation of cross-beam energy transfer. Presented at *49th Annual Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-09. (LA-UR-19-25133)

Yin, L., B. J. Albright, D. J. Stark, W. D. Nystrom and R. F. Bird. Saturation of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams. Presented at *60th Annual Meeting of the APS Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30314)

Posters

Chen, G., L. Chacon, L. Yin, B. J. Albright, D. J. Stark, R. F. Bird and W. D. Nystrom. Optimizations for a semi-implicit, energy- and charge-conserving particle-in-cell algorithm with iVPIC. Presented at *APS DPP annual meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30950)

Search for Axion-mediated Interactions with a Spin-exchange Relaxation-free (SERF) Magnetometer

Young Jin Kim
20180129ER

Project Description

This project will improve the experimental limits of certain axion-mediated spin-dependent interactions over existing experiments, setting new experimental limits on the interaction range below 1 cm. The experimental results will have a profound impact on nuclear physics, astrophysics, and cosmology, and place Los Alamos in the leading position for precision testing of fundamental symmetries and axion searches. This project relies on Los Alamos' expertise in magnetic field sensing to develop new capabilities in fundamental physics and the search for axions. This research will expand the applications of spin-exchange relaxation-free (SERF) magnetometers beyond biophysics.

Technical Outcomes

This project performed the most stringent searches for several axion-mediated exotic interactions between fermions using a spin-exchange relaxation-free (SERF) magnetometer. The experiments set the strongest constraints on the interactions at the centimeter interaction range, narrowing the theoretical bounds, and defined a limit on axion's ability to mediate the interactions. These results demonstrate the feasibility of the innovative high-precision experimental approach and indicate that the experiment will play an important role in exploring the exotic interactions.

Publications

Journal Articles

*Chu, P. -., L. D. Duffy, Y. J. Kim and I. M. Savukov. Sensitivity of proposed search for axion-induced magnetic field using optically pumped magnetometers. 2018. *Physical Review D*. **97** (7): 072011. (LA-UR-18-20811 DOI: 10.1103/PhysRevD.97.072011)

*Chu, P. -., Y. J. Kim and I. Savukov. Search for an axion-induced oscillating electric dipole moment for electrons using atomic magnetometers. 2019. *Physical Review D*. **99** (7): 075031. (LA-UR-18-28540 DOI: 10.1103/PhysRevD.99.075031)

Chu, P., Y. J. Kim, S. G. Newman, I. M. Savukov and J. Long. Experimental search for an exotic spin-spin-velocity-dependent interaction using an optically polarized vapor and a rare earth iron garnet. Submitted to *Physical Review Letters*. (LA-UR-20-27428)

Chu, P., Y. J. Kim and I. M. Savukov. Comment on ”Search for an axion-induced oscillating electric dipole moment forelectrons using atomic magnetometers”. Submitted to *Physical Review D*. (LA-UR-19-23854)

Chu, P., Y. J. Kim and I. M. Savukov. Search for exotic spin-dependent interactions using polarized helium. Submitted to *Physical Review D*. (LA-UR-20-21170)

*Kim, Y. J., P. Chu, I. Savukov and S. Newman. Experimental limit on an exotic parity-odd spin- and velocity-dependent interaction using an optically polarized vapor. 2019. *Nature Communications*. **10** (1): 2245. (LA-UR-19-20817 DOI: 10.1038/s41467-019-10169-1)

*Young, J. K., C. Ping-Han and I. Savukov. Experimental Constraint on an Exotic Spin- and Velocity-Dependent Interaction in the Sub-meV Range of Axion Mass with a Spin-Exchange Relaxation-Free Magnetometer. 2018. *Physical Review Letters*. **121** (9): 091802. (LA-UR-18-22161 DOI: 10.1103/PhysRevLett.121.091802)

Reports

Kim, Y. J. Development of New Directions in Axion Dark Matter Searches. Unpublished report. (LA-UR-19-22470)

Presentation Slides

Chu, P. Dark matter and fundamental physics using atomic magnetometers. Presented at *Telecon for axion dark matter detection*, Los Alamos, New Mexico, United States, 2019-11-26 - 2019-11-26. (LA-UR-19-31565)

Chu, P., Y. J. Kim, I. M. Savukov, S. G. Newman and J. C. Long. Exotic spin-spin-velocity-dependent interaction measurement with a SERF magnetometer and a polarized DyIG sample. Presented at *APS April Virtual Meeting*, Washington, District Of Columbia, United States, 2020-04-18 - 2020-04-21. (LA-UR-20-22885)

Chu, P., Y. J. Kim and I. M. Savukov. Search for an Electron oscillating electric dipole moment using atomic magnetometers. Presented at *APS April 2019*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23004)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. Experimental constraint on an exotic spin- and velocity-dependent interaction with a spin-exchange relaxation-free magnetometer. 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-18-30183)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. New constraints on exotic spin- and velocity-dependent interactions of polarized electrons with an atomic magnetometer. Presented at *APS April Meeting 2019*, Denver, Colorado, United States, 2019-04-12 - 2019-04-16. (LA-UR-19-23005)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. New experimental limits on exotic spin- and velocity-dependent interactions with a spin-exchange relaxation-free atomic magnetometer. Presented at *27th International Nuclear Physics Conference*, Glasgow, United Kingdom, 2019-07-29 - 2019-07-29. (LA-UR-19-27147)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. New constraints on exotic spin- and velocity-dependent interactions of polarized electrons with an atomic magnetometer. Presented at *2019 Fall Meeting of the APS Division of Nuclear Physics*, Crystal City, Virginia, United States, 2019-10-13 - 2019-10-17. (LA-UR-19-30187)

Kim, Y. J., P. Chu and I. M. Savukov. An experimental search for exotic spin-dependent interactions with a spin-exchange relaxation-free magnetometer. Presented at *APS April Meeting*, Columbus, Ohio, United States, 2018-04-14 - 2018-04-14. (LA-UR-18-23132)

Missing Physics behind X-ray Emission from High-Energy-Density Plasmas

Thomas Weber
20180197ER

Project Description

Inertial confinement fusion (ICF) is the one of the most promising concepts for practical fusion energy. Its central idea is imploding a spherical capsule with deuterium-tritium (DT) fuel, which is achieved by ablating its outer layers with high power lasers. In the successful scenario the resulting DT plasma is sufficiently hot and dense to attain and sustain thermo-nuclear burn. While such scenarios are routinely seen in radiation-hydrodynamics (rad-hydro) simulations, their realization in experiments has failed. In the ignition scale experiments the main figure quantifying the implosion performance, the fusion yield, is found much lower than predicted. The key piece of information needed to understand the reasons and cure for this problem is the temperature of the burning plasma. Our project will develop a crucial model which will allow such a temperature diagnostic.

Technical Outcomes

This project developed modeling approaches to evaluate the X-ray emission from Inertial Confinement Fusion (ICF) implosions and obtained theoretical basics for the electron temperature inference. The team also conducted experiments at the Omega laser to validate and improve the models. Solid collaborations with a number of research institutions have been established and the results of the project are expected to affect the temperature diagnostic aspect of the national ICF program.

Publications

Journal Articles

*Kagan, G., O. L. Landen, D. Svyatskiy, H. Sio, N. V. Kabadi, R. A. Simpson, M. G. Johnson, J. A. Frenje, R. D. Petrasso, R. C. Shah, T. R. Joshi, P. Hakel, T. E. Weber, H. G. Rinderknecht, D. Thorn, M. Schneider, D. Bradley and J. Kilkenny. Inference of the electron temperature in inertial confinement fusion implosions from the hard X-ray spectral continuum. 2019. *Contributions to Plasma Physics*. **59** (2): 181-188. (LA-UR-17-28158 DOI: 10.1002/ctpp.201800078)

*Sio, H., J. A. Frenje, A. Le, S. Atzeni, T. J. T. Kwan, M. G. Johnson, G. Kagan, C. Stoeckl, C. K. Li, C. E. Parker, C. J. Forrest, V. Glebov, N. V. Kabadi, A. Bose, H. G. Rinderknecht, P. Amendt, D. T. Casey, R. Mancini, W. T. Taitano, B. Keenan, A. N. Simakov, L. Chacon, S. P. Regan, T. C. Sangster, E. M. Campbell, F. H. Seguin and R. D. Petrasso. Observations of Multiple Nuclear Reaction Histories and Fuel-Ion Species Dynamics in Shock-Driven Inertial Confinement Fusion Implosions. 2019. *Physical Review Letters*. **122** (3): 035001. (LA-UR-18-30435 DOI: 10.1103/PhysRevLett.122.035001)

Properties of Medium Nuclei from First Principles

Stefano Gandolfi
20180210ER

Project Description

This work will enable new algorithms for large scale supercomputing simulations of nuclei and nuclear reactions. Ultimately this work will be valuable for a better description of nuclei and reactions.

Technical Outcomes

This project extended the Auxiliary Field Diffusion Monte Carlo (AFDMC) to include several models of three-body forces in the calculation of nuclear properties, and developed new subroutines to solve for the ground-state of open shell nuclei. The team used the AFDMC code to calculate many properties of nuclei up to oxygen, including energies, radii, spatial and momentum distributions, and others.

Publications

Journal Articles

*Carlson, J. A., A. Lovato, S. Gandolfi, N. Rocco and R. Schiavilla. Study of (v_l, l) and (nubar, l+) Inclusive Scattering in 12C: Confronting the MiniBooNE and T2K CCQE Data. 2020. *Physical Review X*. **10** (3): 31068. (LA-UR-20-22484 DOI: 10.1103/PhysRevX.10.031068)

*Gandolfi, S., D. Lonardoni, A. Lovato and M. Piarulli. Atomic Nuclei From Quantum Monte Carlo Calculations With Chiral EFT Interactions. 2020. *Frontiers*. **8**: 117. (LA-UR-20-20035 DOI: 10.3389/fphy.2020.00117)

*Lonardoni, D., I. Tews, S. Gandolfi and J. A. Carlson. Nuclear and neutron-star matter from local chiral interactions. 2020. *Physical Review Letters*. **2** (2): 022033. (LA-UR-19-32538 DOI: 10.1103/PhysRevResearch.2.022033)

Lynn, J. E., D. Lonardoni, J. A. Carlson, J. W. Chen, W. Detmold, S. Gandolfi and A. Schwenk. Ab initio short-range-correlation scaling factors from light to medium-mass nuclei. Submitted to *Physical Review C*. (LA-UR-19-20911)

Lynn, J., I. Tews, S. Gandolfi and A. Lovato. Quantum Monte Carlo Methods in Nuclear Physics: Recent Advances. Submitted to *Annual Review of Nuclear and Particle Science*. (LA-UR-19-20209)

*Roggero, A. and J. Carlson. Dynamic linear response quantum algorithm. 2019. *Physical Review C*. **100** (3): 034610. (LA-UR-18-22120 DOI: 10.1103/PhysRevC.100.034610)

*Tews, I., J. Margueron and S. Reddy. Confronting gravitational-wave observations with modern nuclear physics constraints. 2019. *The European Physical Journal A*. **55** (6): 97. (LA-UR-19-20198 DOI: 10.1140/epja/i2019-12774-6)

Reports

Gandolfi, S. LDRD Data Sheet. Unpublished report. (LA-UR-19-25844)

Gandolfi, S. Properties of Medium Nuclei from First Principles. Unpublished report. (LA-UR-20-28119)

Presentation Slides

Gandolfi, S., J. A. Carlson and D. Lonardoni. Electron and neutrino scattering from nuclei. . (LA-UR-20-22575)

Classical and Quantum Simulation of Physics

Daniele Spier Moreira Alves
20200604ER

Project Description

This project will advance the theoretical underpinnings required to the development of a fault-tolerant quantum computer. In particular, it will carry over lessons learned from complex physical systems to the development of quantum error correction. This is within the scope of the mission articulated by the Department of Energy (DOE) in its recent Quantum Initiative. Furthermore, quantum information theoretic tools will be used to address challenges in simulating complex physical systems in quantum computers. The goal is to advance the progress and ultimate implementation of such simulations, which will lead to deeper insights into fundamental science of direct relevance to the DOE Office of Science mission, including in High Energy Physics, Nuclear Physics, and Basic Energy Sciences.

Technical Outcomes

This project proved bounds on quantum field digitization and studied a full classical/quantum simulation algorithm for strongly coupled scalar field theory. The research also developed new low-energy ansatz states of quantum field theories that improve the efficiency of quantum simulations of the dynamics of these systems in low-energy subspaces of the full Hilbert space.

Publications

Journal Articles

Somma, R. D. and M. B. Sahinoglu. Hamiltonian simulation in the low energy subspace. Submitted to *Physical Review Letters*. (LA-UR-20-23338)

Research into Advanced Methods for Sensitivity Analysis, Gap Analysis, and Experiment Optimization for Weapons, Nuclear Energy, and Global Security Applications

Jesson Hutchinson
20200620ER

Project Description

Radiation transport simulations are used for all aspects of the nuclear industry including defense programs, nonproliferation, counterproliferation, nuclear energy, space applications (National Aeronautics and Space Administration), criticality safety, medical physics, and others. These simulations require nuclear data, therefore accurate nuclear data is essential to produce accurate results. This work will result in the design of new critical and subcritical experiments which will ultimately lead to nuclear data improvements for relevant applications. As nuclear data improves, the understanding of device performance and criticality will also be improved. This work will require recent and new simulation tools and will result in better understanding of cross-section sensitivities for systems which are very relevant to the weapons and nonproliferation programs. The experiments will be designed for the National Criticality Experiments Research Center (but experiment execution is outside the scope of this project and is part of the future work).

Technical Outcomes

Technical outcomes for this project included new optimization capabilities, tools for time and energy-dependent sensitivities, a tool for nuclear data library comparison for compensating error identification, a keff filter for experiment optimization, and an investigation of experiment uncertainties.

Publications

Conference Papers

Hutchinson, J. D., J. L. Alwin, T. J. Grove, I. J. Michaud, T. A. Smith, R. C. Little, N. A. Kleedtke, M. E. Rising and N. W. Thompson. Sensitivity Studies, Gap Analysis, and Benchmark Experiment Optimization for Reactor Physics and Criticality Safety Applications. Presented at *ANS Winter Conference*. (Chicago, Illinois, United States, 2020-11-16 - 2020-11-16). (LA-UR-20-24750)

Kleedtke, N. A., I. J. Michaud, M. E. Rising, T. J. Grove, J. D. Hutchinson and B. C. Kiedrowski. Gaussian Process Optimization of Sensitivity-Based Similarity Metrics between New Nuclear Applications and New/Existing Benchmarks. Presented at *American Nuclear Society Winter Meeting and Expo*. (Chicago, Illinois, United States, 2020-11-15 - 2020-11-19). (LA-UR-20-24718)

Presentation Slides

Hutchinson, J. D., I. J. Michaud, R. C. Little, J. L. Alwin, T. J. Grove, A. T. McSpaden, M. E. Rising, T. A. Smith and N. W. Thompson. The Los Alamos ARCHIMEDES Project: Application-specific experiments for nuclear data and analytical methods validation. Presented at *WANDA Meeting*, Washington DC, District Of Columbia, United States, 2020-03-03 - 2020-03-03. (LA-UR-20-22212)

New Theoretical and Computational Capabilities for the Astrophysical Multi-Messenger Era

Hui Li
20200661ER

Project Description

Multi-messenger astrophysics is a rapidly developing field and Los Alamos can take a leadership role in theory and modeling with our unique capabilities. It addresses some of the fundamental questions in science by developing state-of-the-art numerical simulation tools that will become useful to Los Alamos missions. This work will sustain the development of a core capability at Los Alamos in astrophysics, which has also served as an effective pipeline for high-quality scientists.

Technical Outcomes

This project helped develop a new physics package for Los Alamos' Vector Particle-In-Cell (VPIC) code, addressing challenging problems in astrophysical particle acceleration in multi-messenger astrophysics. The team studied how binary black holes will evolve in disks, which undergirds our modeling of electromagnetic counterparts associated with gravitational wave emissions. The team also obtained new solutions of the Einstein's equations for a slowly rotating gravastar to second order in the ratio of angular momentum of the black hole to its mass.

Publications

Journal Articles

Chen, Y., X. Zhang, Y. Li, H. Li and D. Lin. Retention of Long-Period Gas Giant Planets: Type II Migration Revisited. Submitted to *Astrophysical Journal*. (LA-UR-20-24009)

*Chen, Y., Y. Li, H. Li, D. N. Lin and D. N. Lin. The Preservation of Super-Earths and the Emergence of Gas Giants after Their Progenitor Cores Have Entered the Pebble-isolation Phase. 2020. *The Astrophysical Journal*. **896** (2): 135. (LA-UR-20-22160 DOI: 10.3847/1538-4357/ab9604)

Dempsey, A. M., Y. Lithwick and D. Mu\xc3\xb1oz. Outward Planet Migration in Gapped, Eccentric Disks. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-29630)

Guo, F., X. Li, W. S. Daughton, H. Li, P. F. H. Kilian, Y. H. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics and Particle Acceleration during Relativistic Turbulent Magnetic Reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-26005)

Guo, F., Y. Liu, X. Li, H. Li, W. S. Daughton and P. F. H. Kilian. Recent Progress on Particle Acceleration and Reconnection Physics during Magnetic Reconnection in the Magnetically-dominated Relativistic Regime. Submitted to *Physics of Plasmas*. (LA-UR-20-26135)

*Laune, J. T., L. Hui, L. Shengtai, L. Ya-Ping, L. G. Walls, T. Birnstiel, J. Drazdotkowska and S. Stammler. Ring Morphology with Dust Coagulation in Protoplanetary Disks. 2020. *The Astrophysical Journal*. **889** (1). (LA-UR-20-28596 DOI: 10.3847/2041-8213/ab65c6)

Li, J., A. M. Dempsey, H. Li and S. Li. Rings Formation by Unstable Eccentric modes in Disks with Cooling. Submitted to *Astrophysical Journal*. (LA-UR-20-27570)

Li, Y., A. M. Dempsey, S. Li, H. Li and J. Li. Orbital evolution of binary black hole in active galactic nucleus disks: a disk channel for binary black hole mergers?. Submitted to *Astrophysical Journal*. (LA-UR-20-28080)

Li, Y., Y. Chen, D. N. C. Lin and X. Zhang. Accretion of Gas Giants Constrained by the Tidal Barrier. 2021. *The Astrophysical Journal*. **906** (1): 52. (LA-UR-20-26761 DOI: 10.3847/1538-4357/abc883)

Lyu, F., Y. Li, S. Hou, J. Geng, X. Wu and E. Liang. Self-organized Criticality in Multi-pulse Gamma-Ray Bursts. Submitted to *Nature Astronomy*. (LA-UR-20-23425)

Zhang, H., X. Li, D. Giannios, F. Guo, Y. H. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–I. A. Submitted to *Astrophysical Journal*. (LA-UR-20-27998)

zhang, h., X. Li, F. Guo and D. Giannios. First-Principle Prediction of X-ray Polarization from Magnetic Reconnection in High-Frequency BL Lacs. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-30074)

Reports

Li, Y. Report for IC proposal: Exploring Planet-disk Interaction in Dusty Protoplanetary Disks and Their Observational Implications. Unpublished report. (LA-UR-21-21683)

Presentation Slides

Guo, F. Particle Acceleration in Magnetic Reconnection: From Small Scale to Large Scale. Presented at *2020 Magnetic Reconnection Workshop*, Weihai, China, 2020-08-24 - 2020-08-25. (LA-UR-20-26501)

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)

H. Kilian, P. F., X. Li, F. Guo and H. Li. Exploring the acceleration mechanisms for particle injection and power-law formation during trans-relativistic magnetic reconnection. Presented at *Understanding the Most Energetic Cosmic Accelerators: Advances in Theory and Simulation*, Online, New Mexico, United States, 2020-10-28 - 2020-10-30. (LA-UR-20-28623)

Li, Y. Gas/Dust Dynamics, Planet Formation in Protoplanetary Disks and the Possible Applications. Presented at *Seminar at Shanghai Astronomical Observatory*, Online, New Mexico, United States, 2020-12-23 - 2020-12-23. (LA-UR-20-30385)

Li, Y. IC project: Exploring Planet-disk Interaction in Dusty Protoplanetary Disks and Their Observational Implications. . (LA-UR-21-20119)

Li, Y. Embedded binary black holes in AGN disks. Presented at *talk at University of Nevada, Las Vegas*, Online, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21914)

Li, Y., A. M. Dempsey, S. Li, H. Li and J. Li. Orbital evolution of binary black holes in active galactic nucleus disks: a disk channel for binary black hole mergers?. Presented at *The 36th Annual New Mexico Symposium*, Online, New Mexico, United States, 2020-11-13 - 2020-11-13. (LA-UR-20-29419)

Li, Y., A. M. Dempsey, S. Li, H. Li and J. Li. An AGN disk channel for binary black hole mergers. Presented at *Los Alamos \xc2\xa0Astrophysics Seminar Series*, Online, New Mexico, United States, 2021-02-18 - 2021-02-18. (LA-UR-21-21492)

Li, Y., H. Li, S. Li, T. Birnstiel, J. Drazkowska and S. Stammler. The impact of dust growth on the observed sub-structures in protoplanetary disks. Presented at *American Astronomical Society 236th*, Online, New Mexico, United States, 2020-06-01 - 2020-06-03. (LA-UR-20-23968)

Li, Y., Y. Chen, D. Lin, X. Zhang and H. Li. Preservation of Super-Earths in Protoplanetary Disks. Presented at *Earth-2.0 workshop*, Online, New Mexico, United States, 2020-10-28 - 2020-10-29. (LA-UR-20-28689)

Posters

Li, Y., H. Li, S. Li, J. T. Laune, T. Birnstiel, J. Dra\xcc\xa7\xc5\xbckowska and S. Stammler. Effect of Dust Coagulation on the Sub-structures in Protoplanetary Disks. Presented at *Planetesimal formation meeting*, Online, New Mexico, United States, 2020-11-17 - 2020-11-17. (LA-UR-20-29420)

Li, Y., H. Li, S. Li, J. T. Laune, T. Birnstiel, J. Dra\xcc\xa7\xc5\xbckowska and S. Stammler. Effect of Dust Coagulation on the Sub-structures in Protoplanetary Disks. Presented at *Five years after HL Tau: a new era in planet formation*, Online, New Mexico, United States, 2020-12-07 - 2020-12-11. (LA-UR-20-29930)

Li, Y., H. Li, S. Li and D. N. L. Lin. Dust Signatures Induced by Eccentric Super-Earths in Protoplanetary Disks. Presented at *Five years after HL Tau: a new era in planet formation*, Online, New Mexico, United States, 2020-12-07 - 2020-12-11. (LA-UR-20-30046)

Li, Y., Y. Chen, D. Lin and X. Zhang. Accretion of Gas Giants Constrained by the Tidal Barrier. Presented at *Exoplanets in Southern California 2020 conference*, Online, California, United States, 2020-09-14 - 2020-09-15. (LA-UR-20-27384)

Developing Dark Matter Detectors from Novel Narrow Band Gap Materials

Daniele Spier Moreira Alves
20200751ER

Project Description

About 85% of the total mass in the Universe consists of dark matter, but very little has been established about its properties. New technology that could detect light dark matter particles would have a transformative science impact, and is a high priority for the Department of Energy's Office of Science. This project will deliver the results of feasibility studies of a new detection technology concept to probe dark matter particles lighter than the electron. This pioneering capability could have further potential applicability in other areas of relevance to national priorities, such as quantum sensing of single photons from far infrared to ultraviolet.

Technical Outcomes

This project delivered preliminary studies to assess the feasibility of a novel detection concept for light dark matter based on narrow gap semiconductors discovered at Los Alalmos. Experimentally, the team synthesized single crystals of LaCdAs2 and Eu5In2Sb6 and measured their current-voltage (I-V) characteristics at liquid helium temperatures. Theoretically, the team evaluated the band structure and dielectric function of these materials via density functional theory calculations and estimated the sensitivity of Eu5In2Sb6 to dark matter absorption signals.

Publications

Presentation Slides

Spier Moreira Alves, D. Quantum Materials for Dark Matter Detection. Presented at *Presentation for meeting with T-DO about joint T-2/T-4 efforts in Quantum Materials*, Los Alamos, New Mexico, United States, 2020-12-22 - 2020-12-22. (LA-UR-20-30422)

Path to High-energy Proton Radiography (pRAD) Upgrade at the Los Alamos Neutron Science Center (LANSCE)

John Lewellen
20200764ER

Project Description

Dynamic imaging capabilities, such as proton radiography, provide a wealth of information relevant to both stockpile stewardship and design of future capabilities. This project will explore a concept for dramatically improving the capabilities of proton radiography, specifically by taking advantage of recent advances in accelerator technology. High-accelerating-field, cryogenically cooled copper accelerator structures offer the promise of factors of 10 improvement in resolution, and experiments much closer to "full-scale" than can presently be accommodated at our existing facilities.

Technical Outcomes

This project explored the possibility of using high-accelerating-field copper accelerator structures to accelerate a proton beam beyond the end of the existing Los Alamos Neutron Science Center (LANSCE) linac, from the standpoints of beam quality preservation and transport to much higher energies. The simulations indicate that it is indeed possible to use advanced structures, providing 100-200 times the acceleration of existing LANSCE structures, to accelerate a proton beam for proton radiography.

A Multidimensional Multiscale Vlasov-Fokker-Planck Algorithm for Modeling High Energy Density and Inertial Confinement Fusion Applications

William Taitano
20190529ECR

Project Description

After the failed attempt of ignition at the National Ignition Facility (NIF), the predictive capabilities of our radiation hydrodynamic (rad-hydro) codes have been put into question. At the moment, it is not clear if the mismatch between calculations and experiments is caused by missing physics (e.g., kinetic plasma effects) in our rad-hydro codes, or inferior algorithms used therein. The project will build foundational algorithmic capabilities which will allow us to investigate the role of these 'missing physics' in our rad-hydro simulations and ultimately, increase our predictive capabilities for related laboratory experiments.

Publications

Reports

Taitano, W., L. Chacon and A. N. Simakov. The Annual IC Progress Report. Unpublished report. (LA-UR-20-22359)

Presentation Slides

Taitano, W. A Multiscale Eulerian Vlasov-Fokker-Planck Algorithm with Applications to High Energy Density Systems. Presented at *Virtual seminar at the Air Force Research Laboratory*, Los Alamos, New Mexico, United States, 2021-02-01 - 2021-02-01. (LA-UR-21-20616)

Posters

Taitano, W. A Conservative Multiscale 2D3V Curvilinear Phase-Space Moving Grid Algorithm for the Vlasov Equation with Applications to High Energy Density System. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics (Virtual Meeting)*, Los Alamos, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29145)

Adaptive Process Control for Beyond-State-of-the-Art Alkali Antimonide Photocathodes

Vitaly Pavlenko
20190536ECR

Project Description

Hard X-ray free electron lasers such as Linac Coherent Light Source-II (LCLS-II) and Matter-Radiation Interactions in Extremes (MaRIE) are considered essential to enable sustainable stockpile stewardship. Reliable operation and performance of such billion-dollar facilities depends on a tiny but critical piece, a photocathode (laser-triggered source of electrons). Fabrication of one of the most important photocathode types, alkali antimonides, to this day remains an art, as opposed to a technological process that applies to every other part of the system. We believe that we possess the knowledge required to eliminate the vulnerability and poor reproducibility associated with a human-controlled process and deliver the first-ever fully automated photocathode growth system.

Publications

Journal Articles

Alexander, A. M., M. Gaowei, S. Mistry, J. Walsh, F. Liu, K. Evans-Lutterdot, E. Stavitski, V. Pavlenko, K. Attenkofer, J. M. Smedley and N. A. Moody. Robust method for broadband efficiency enhancement of electron photocathodes using optical interferences. Submitted to *Applied Physics Letters*. (LA-UR-21-22492)

Posters

Alexander, A. M., F. Liu, V. Pavlenko, N. A. Moody, J. M. Smedley and P. Bandaru. Interference Enhanced Photocathodes. Presented at *Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28528)

A Dual n-gamma Detector Array to Correct Neutron Transport Simulations

Keegan Kelly
20190588ECR

Project Description

Monte Carlo simulations of nuclear systems are essential for the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) national nuclear security missions. These simulations contain ambiguities because they include commonly-encountered neutron scattering cross sections that are poorly known, poorly measured, and estimated from nuclear models. This project aims to resolve these ambiguities by taking advantage of recent developments in detector technologies to create a detector system capable of yielding accurate and complete measurements of these cross sections and the corresponding angular distributions.

Publications

Journal Articles

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., M. J. Devlin and J. M. O'Donnell. Development of a Highly-Segmented Dual n-gamma Detector Array for Neutron Scattering Measurements at LANL. Presented at *SORMAWest 2020*. (Berkeley, California, United States, 2020-06-01 - 2020-06-04). (LA-UR-20-21042)

Presentation Slides

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)

Resolving Transport Processes in Multispecies Plasma Shock Waves

Samuel Langendorf
20200564ECR

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.

Exploring Inside the Los Alamos Neutron Science Center (LANSCE) Hydrogen- Ion Source with Laser Absorption Techniques

David Kleinjan
20200570ECR

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.

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)

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)

Quantum Chromodynamics (QCD) Fragmentation Scaling Laws from Space-Time Reciprocity

Duff Neill
20200584ECR

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.

Publications

Journal Articles

Neill, D. A. Local Parton-Hadron Duality Revisited. Submitted to *Journal of High Energy Physics*. (LA-UR-20-27861)

Kinetic Study of a Magnetic-Mirror Wet-Wood-Burner Fusion Neutron Source

Ari Le
20200587ECR

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.

Publications

Journal Articles

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., 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)

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

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)

Integrated Study of X-ray Free-electron Lasers (XFEL) Performance with High Brightness Bunched Electron Beams

Petr Anisimov
20180535ECR

Project Description

There is a strong national need for high quality light sources at hard x-rays to dynamically image high-Z materials used in nuclear weapons and examine materials in extreme conditions. This work addresses the challenges of dynamic materials performance and process aware manufacturing. X-ray free electron lasers operating at a coherent photonic energy gap of the 42+keV (kiloelectron volts) region will be used to study multiphase high explosive evolution; dynamic performance of plutonium, surrogate metals, and alloys; turbulent material mixing in variable density flows; and controlled solidification and phase transformations, predicting interfacial microstructure and strain evolution, and aiding high explosive functionality by design.

Technical Outcomes

This LDRD project developed the Laser Assisted Bunch Compression (LABC) scheme for high brightness, high current electron beams to be used in 42+keV (kiloelectron volts) X-ray free electron lasers (XFELs). The team numerically demonstrated that the LABC compression scheme solves the critical problem currently hindering the performance of the 42+keV XFELs and enables an ultra-compact XFEL design for university campuses. The project has also led to follow-on funding for experimental testing of the developed compression scheme.

Publications

Journal Articles

Anisimov, P. M., B. E. Carlsten, C. W. Barnes, Q. R. Marksteiner, R. R. Robles and N. Yampolsky. High-Brightness Beam Technology Development for a Future Dynamic Mesoscale Materials Science Capability. 2019. *Instruments*. **3** (4): 52. (LA-UR-20-29585 DOI: 10.3390/instruments3040052)

Carlsten, B. E., P. M. Anisimov, C. W. Barnes, Q. R. Marksteiner, R. R. Robles and N. Yampolsky. High-Brightness Beam Technology Development for a Future Dynamic Mesoscale Materials Science Capability. 2019. *Instruments*. **3** (4): 52. (LA-UR-19-28549 DOI: 10.3390/instruments3040052)

*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)

Presentation Slides

Anisimov, P. M. High-Efficiency Free Electron Lasers with Pinched Electron Beams. Presented at *Physics & Applications of High Efficiency Free-Electron Lasers Workshop*, Los Angeles, California, United States, 2018-04-11 - 2018-04-13. (LA-UR-18-23463)

Anisimov, P. M., Q. R. Marksteiner, R. R. Robles, J. W. I. Lewellen, N. Yampolsky and B. E. Carlsten. Laser Assisted Bunch Compression for High Energy X-ray Free Electron Lasers. Presented at *FEL 2019*, Hamburg, Germany, 2019-08-26 - 2019-08-30. (LA-UR-19-28673)

Carlsten, B. E. Accelerator Challenges for XFELs with Very High X-Ray Energies. Presented at *39th International Free-Electron Laser Conference*, Hamburg, Germany, 2019-08-26 - 2019-08-30. (LA-UR-19-28626)

Posters

Robles, R. R., J. E. Williams and P. M. Anisimov. Increasing High-Energy XFEL Efficiency with a Transverse Gradient Undulator. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-26791)

Critical Analysis of Neutrinoless Double Beta Decay with Effective Field Theories

Emanuele Mereghetti
20180573ECR

Project Description

Neutrinos are fascinating, elusive elementary particles, and the understanding of their properties holds the keys to answering fundamental open questions in particle physics, such as the origin of matter-antimatter asymmetry in the universe. A particularly pressing question is whether neutrinos are their own antiparticles, which would imply that at a fundamental level "matter number" is not conserved in nature. The definitive answer to this question will come from the observation of neutrinoless double beta decay, an extremely rare nuclear process. The importance of this process is stressed by the decision of the US Nuclear Physics community to identify in the Nuclear Science Advisory Committee's 2015 Long Range Plan “the timely development and deployment of a US-led ton-scale neutrinoless double beta decay experiment” as the highest priority for new projects across all the subfields of nuclear physics. By critically examining the theoretical uncertainties that affect double beta decay, and by developing a very general framework for the interpretation of double beta decay searches, our project will strengthen the case for such a high-profile Department of Energy endeavor.

Technical Outcomes

This project developed a unified description of neutrinoless double beta decays (0nbb) in Effective Field Theories (EFT). The team derived the transition operator in chiral EFT, discovered a new leading-order contribution that had been missed in all the existing literature. The team derived a master formula, applicable to all models of lepton-number-violation, with consistent hadronic and nuclear theory input. The project started collaborations with theorists in the lattice-quantum chromodynamics (QCD) and nuclear structure communities, to achieve controlled calculations of 0nbb matrix elements.

Publications

Journal Articles

*Alioli, S., W. Dekens, M. Girard and E. Mereghetti. NLO QCD corrections to SM-EFT dilepton and electroweak Higgs boson production, matched to parton shower in POWHEG. 2018. *Journal of High Energy Physics*. **2018** (8): 205. (LA-UR-18-23399 DOI: 10.1007/JHEP08(2018)205)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser, E. Mereghetti, S. Pastore and U. van Kolck. New Leading Contribution to Neutrinoless Double-\xce\xb2 Decay. 2018. *Physical Review Letters*. **120** (20): 202001. (LA-UR-18-21404 DOI: 10.1103/PhysRevLett.120.202001)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser and E. Mereghetti. A neutrinoless double beta decay master formula from effective field theory. 2018. *Journal of High Energy Physics*. **2018** (12): 97. (LA-UR-18-24895 DOI: 10.1007/JHEP12(2018)097)

Mereghetti, E., A. Walker-Loud, C. Drischler, A. N. Nicholson, W. Haxton, K. McElvain and P. Vranas. Towards grounding nuclear physics in QCD. 2020. *European Physical Journal A. Hadrons and Nuclei*. 103822. (LA-UR-19-30583 DOI: 10.1016/j.ppnp.2020.103822)

*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)

Mereghetti, E., V. Cirigliano, W. G. Dekens, J. de Vries, M. L. Graesser, S. Pastore, M. Piarulli, U. Van Kolck and R. B. Wiringa. A renormalized approach to neutrinoless double beta decay. Submitted to *Physical Review C*. (LA-UR-19-26002)

*Wang, X. B., A. C. Hayes, J. Carlson, G. X. Dong, E. Mereghetti, S. Pastore and R. B. Wiringa. Comparison between variational Monte Carlo and shell model calculations of neutrinoless double beta decay matrix elements in light nuclei. 2019. *Physics Letters B*. **798**: 134974. (LA-UR-19-25587 DOI: 10.1016/j.physletb.2019.134974)

Conference Papers

Mereghetti, E. Lattice QCD and nuclear physics for searches of physics beyond the Standard Model. Presented at *36th Annual International Symposium on Lattice Field Theory*. (Lansing, Michigan, United States, 2018-07-22 - 2018-07-28). (LA-UR-18-30382)

Presentation Slides

Mereghetti, E. Electric dipole moments of light nuclei. Presented at *Atomic Nuclei as Laboratories for BSM physics*, Trento, Italy, 2019-04-15 - 2019-04-19. (LA-UR-19-30719)

Mereghetti, E. An Effective Field Theory Approach to neutrinoless double beta decay. . (LA-UR-19-30720)

Mereghetti, E. Constraining BSM physics with hadronic and nuclear physics. Presented at *Hadron 2019*, Guilin, China, 2019-08-16 - 2019-08-21. (LA-UR-19-28353)

New Physics at the Giga Electron Volt (GeV) Scale, with Implications for the Strong Charge-conjugation x Parity (CP) Problem

Daniele Spier Moreira Alves
20180622ECR

Project Description

The high level goal is to explore new dynamics that addresses puzzling properties of the neutron and of the strong interactions, and its implications for the structure of matter and forces, the Higgs boson, and neutrinos. The expected outcome is a further understanding of the role of beyond the Standard Model physics in Giga Electron Volt (GeV) scale dynamics, which could lead to new experimental opportunities and discoveries, directly impacting the mission of the Department of Energy Office of Science. This project addresses the challenges defined as high priority scientific goals by the 2014 DOE Particle Physics Project Prioritization Panel (a subpanel of the High Energy Physics Advisory Panel), the 2015 DOE Nuclear Physics Long-Range Plan, and the Laboratory's fiscal year 2018 (FY18) Strategic Investment Plan, specifically in its Nuclear and Particle Futures pillar.

Technical Outcomes

The team explained anomalies in nuclear transitions via axion emission in a viable implementation of Peccei-Quinn mechanism at giga-electron volt (GeV) scale. If confirmed, this would be transformational in two aspects: as a discovery of an elementary particle, and as a solution to the "Strong CP Problem." The research calculated predictions for axion signals that could be verified within the next decade in upcoming meson factories and in nuclear reactions that could be measured at Los Alamos.

Publications

Journal Articles

Spier Moreira Alves, D. Signals of the QCD axion with mass of 17 MeV/c2: nuclear transitions and light meson decays. Submitted to *Journal of High Energy Physics*. (LA-UR-20-27039)

Presentation Slides

Spier Moreira Alves, D. Signals of the QCD axion with mass of 17 MeV. . (LA-UR-20-28286)

Spier Moreira Alves, D. New Physics Signals In Hadronic Processes. . (LA-UR-21-22706)

Mega Electron Volt (MeV) Gamma-Ray Astronomy: Exploring the Universe in the Nuclear Transition Region

Lucas Parker
20170693PRD4

Project Description

The development of more sensitive space-based instruments for the detection of gamma-ray and neutron emission generated by nuclear reactions is important for Department of Energy/National Nuclear Security Administration national security programs. This project will develop new tools for imaging sources of gamma-ray and neutron emission that will allow the detection and measurement of sources that are currently too faint to detect. The project will also explore new approaches to the reduction of detector background noise that will enable the construction of more sensitive gamma-ray and fast neutron detectors. Our development of these new tools for on-board Compton gamma-ray imaging and background reduction is likely to influence future designs of Space-based Nuclear Detonation Detection (SNDD) instrumentation.

Publications

Journal Articles

*Appel, J. W., Z. Xu, I. L. Padilla, K. Harrington, B. Pradenas Marquez, A. Ali, C. L. Bennett, M. K. Brewer, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. Couto, S. Dahal, K. Denis, R. Dunner, J. R. Eimer, T. Essinger-Hileman, P. Fluxa, D. Gothe, G. C. Hilton, J. Hubmayr, J. Iuliano, J. Karakla, T. A. Marriage, N. J. Miller, C. Nunez, L. Parker, M. Petroff, C. D. Reintsema, K. Rostem, R. W. Stevens, D. A. N. Valle, B. Wang, D. J. Watts, E. J. Wollack and L. Zeng. On-sky Performance of the CLASS Q-band Telescope. 2019. *The Astrophysical Journal*. **876** (2): 126. (LA-UR-18-30124 DOI: 10.3847/1538-4357/ab1652)

*Kusaka, A., J. Appel, T. Essinger-Hileman, J. A. Beall, L. E. Campusano, H. Cho, S. K. Choi, K. Crowley, J. W. Fowler, P. Gallardo, M. Hasselfield, G. Hilton, S. P. Ho, K. Irwin, N. Jarosik, M. D. Niemack, G. W. Nixon, M. Nolta, L. A. J. Page, G. A. Palma, L. Parker, S. Raghunathan, C. D. Reintsema, J. Sievers, S. M. Simon, S. T. Staggs, K. Visnjic and K. Yoon. Results from the Atacama B-mode Search (ABS) experiment. 2018. *Journal of Cosmology and Astroparticle Physics*. **2018** (09): 5-5. (LA-UR-18-23879 DOI: 10.1088/1475-7516/2018/09/005)

Parker, L. P., S. Dahal, M. K. Brewer, A. Ali, J. W. Appel, C. L. Bennett, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. D. Couto, R. Datta, K. L. Denis, J. Eimer, F. Espinoza, T. Essinger-Hileman, D. Gothe, K. Harrington, J. Iuliano, T. A. Marriage, S. Novack, C. Nunez, I. L. Padilla, M. Petroff, R. Reeves, G. Rhoades, K. Rostem, D. A. N. Valle, D. J. Watts, E. J. Wollack and Z. Xu. Venus Observations at 40 and 90 GHz with CLASS. Submitted to *Planetary Science Journal*. (LA-UR-20-28472)

Parker, L. P., Z. Li, S. Naess, S. Aiola, J. W. Appel, R. J. Bond, E. Calabrese, S. K. Choi, T. Essinger-Hileman, J. Dunkley, J. Fowler, P. Gallardo, J. Hubmayr, M. D. Niemack, L. Page, B. Partridge, M. Salatino, C. Sifon, S. M. Simon, S. T. Staggs, E. Storer and E. Wollack. The Cross Correlation of the ABS and ACT Maps. Submitted to *Astrophysical Journal*. (LA-UR-20-21154)

*Watts, D. J., B. Wang, A. Ali, J. W. Appel, C. L. Bennett, D. T. Chuss, S. Dahal, J. R. Eimer, T. Essinger-Hileman, K. Harrington, G. Hinshaw, J. Iuliano, T. A. Marriage, N. J. Miller, I. L. Padilla, L. Parker, M. Petroff, K. Rostem, E. J. Wollack and Z. Xu. A Projected Estimate of the Reionization Optical Depth Using the CLASS Experiment's Sample Variance Limited E-mode Measurement. 2018. *The Astrophysical Journal*. **863** (2): 121. (LA-UR-18-20165 DOI: 10.3847/1538-4357/aad283)

Conference Papers

Dahal, S., A. Ali, J. W. Appel, T. Essinger-Hileman, C. Bennett, M. Brewer, R. Bustos, M. Chan, D. Chuss, J. Cleary, T. Engelhoven, P. Fluxa, F. Colazo, J. Couto, K. Denis, R. Dunner, J. Eimer, M. Halpern, K. Harrington, K. Helson, G. Hilton, G. Hinshaw, J. Hubmayr, J. Iuliano, J. Karakla, B. Marquez, T. Marriage, J. McMahon, N. Miller, C. Nunez, I. Padilla, G. Palma, L. P. Parker, M. Petroff, R. Reeves, C. Reintsema, K. Rostrem, M. Sagliocca, K. U-Yen, D. Valle, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan and L. Zeng. Design and Characterization of Cosmology Large Angular Scale Surveyor (CLASS) 93 GHz Focal Plane. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-24478)

Harrington, K., J. Eimer, D. Chuss, M. Petroff, J. Cleary, M. DeGeorge, A. Ali, J. W. Appel, C. Bennett, M. Brewer,

R. Bustos, M. Chan, J. Couto, K. Denis, R. Dunner, T. Essinger-Hileman, P. Fluxa, M. Halpern, G. Hilton, G. Hinshaw, J. Hubmayr, J. Iuliano, J. Karakla, T. Marriage, J. McMahon, N. Miller, C. Nunez, I. Padilla, G. Palma, L. P. Parker, B. Marquez, R. Reeves, C. Reintsema, K. Rostem, D. Valle, T. Engelhoven, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan and L. Zeng. Variable-delay Polarization Modulators for the CLASS Telescopes. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-24622)

Iuliano, J., J. Eimer, L. P. Parker, A. Ali, J. W. Appel, C. Bennett, M. Brewer, R. Bustos, D. Chuss, J. Cleary, J. Couto, S. Dahal, K. Denis, R. Dunner, T. Essinger-Hileman, P. Fluxa, M. Halpern, K. Harrington, K. Helson, G. Hilton, G. Hinshaw, J. Hubmayr, J. Karakla, T. Marriage, N. Miller, J. McMahon, C. Nunez, I. Padilla, G. Palma, M. Petroff, B. Marquez, R. Reeves, C. Reintsema, K. Rostrem, D. Valle, T. Engelhoven, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan and L. Zeng. The Cosmology Large Angular Scale Surveyor Receiver Design. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-25031)

Parker, L. P., S. Griffin, C. Kierans, A. Schoenwald, P. Shawhan, R. Caputo, J. McEnery and J. Perkins. Current Status of the ComPair Silicon Tracker. Presented at *SPIE Astronomical Telescopes + Instrumentation (digital, remote)*. (Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16). (LA-UR-20-29832)

Presentation Slides

Parker, L. P. An FPGA-based Compton Mapping Pipeline. . (LA-UR-20-30237)

Posters

Parker, L. P., S. Grifffin, C. Kierans, A. Shoenwald, P. Shawhan, R. Caputo, J. McEnery and J. Perkins. Progress towards the Silicon Tracker for the All-sky Medium Energy Gamma-ray Observatory Prototype. Presented at *IEEE Nuclear Science Symposium (NSS) and Medical Imaging Conference (MIC)*, Manchester, United Kingdom, 2019-10-26 - 2019-11-02. (LA-UR-19-30803)

Conservative Slow-Manifold Integrators

Joshua Burby
20180756PRD4

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.

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., J. Finn and C. L. Ellison. Improved accuracy in degenerate variational integrators for guiding center and magnetic field line flow. Submitted to *Journal of Plasma Physics*. (LA-UR-21-22168)

Burby, J. W., N. Duignan and J. Meiss. Integrability, normal forms and magnetic axis coordinates. Submitted to *Journal of Mathematical Physics*. (LA-UR-21-22030)

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)

Burby, J. W., N. Kallinikos and R. S. MacKay. Some mathematics for quasi-symmetry. Submitted to *Journal of Mathematical Physics*. (LA-UR-19-32407)

Burby, J. W., R. L. Dewar, Z. S. Qu, N. Sato and M. J. Hole. Time-dependent relaxed magnetohydrodynamics -- inclusion of cross helicity constraint using phase-space action. Submitted to *Physics of Plasmas*. (LA-UR-20-23641)

Burby, J. W., R. MacKay and N. Kallinikos. Approximate symmetries of guiding-centre motion. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-20-28555)

*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 J. Squire. General formulas for adiabatic invariants in nearly-periodic Hamiltonian systems. Submitted to *Journal of Plasma Physics*. (LA-UR-20-23640)

Burby, J. W. and T. J. Klotz. INVITED: Slow manifold reduction for plasma science. 2020. *Communications in Nonlinear Science and Numerical Simulation*. **89**: 105289. (LA-UR-19-32243 DOI: 10.1016/j.cnsns.2020.105289)

*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)

*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)

Reports

Klotz, T. and J. W. Burby. Slow Manifolds of fast-slow systems, the Vlasov-Maxwell System, and Control of Confined Plasma. Unpublished report. (LA-UR-19-27827)

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., N. Kallinikos and R. MacKay. Grad-Shafranov equation for non-axisymmetric MHD equilibria. . (LA-UR-20-24872)

Burby, J. W., Q. Tang and R. Maulik. Computing Poincare maps using physics-informed deep learning. . (LA-UR-20-25536)

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)

Matter and Nuclei at Neutron-Rich Extremes

Ingo Tews
20190617PRD1

Project Description

The work will involve large-scale calculations of atomic nuclei and of dense nucleonic matter present in neutron stars. Advancing our ability to calculate the properties and reactions of atomic nuclei will allow us to advance the state of the art in predicting nuclear reactions in regimes where experiments are difficult or impossible, like reactions on unstable nuclei.

Publications

Journal Articles

Al-Mamun, M., A. W. Steiner, J. Nattila, J. Lange, R. O'Shaughnessy, I. Tews, S. Gandolfi, C. Heinke and S. Han. Combining Electromagnetic and Gravitational-Wave Constraints on Neutron-Star Masses and Radii. Submitted to *Physical Review Letters*. (LA-UR-20-26423)

*Capano, C. D., I. Tews, S. M. Brown, B. Margalit, S. De, S. Kumar, D. A. Brown, B. Krishnan and S. Reddy. Stringent constraints on neutron-star radii from multimessenger observations and nuclear theory. 2020. *Nature Astronomy*. **4** (6): 625-632. (LA-UR-19-28442 DOI: 10.1038/s41550-020-1014-6)

Dietrich, T., M. W. Coughlin, P. T. H. Pang, M. Bulla, J. Heinzel, L. Issa, I. Tews and S. Antier. New Constraints on the Supranuclear Equation of State and the Hubble Constant from Nuclear Physics--Multi-Messenger Astronomy. Submitted to *Science*. (LA-UR-20-21470)

Essick, R. C., P. Landry, A. Schwenk and I. Tews. A Detailed Examination of Astrophysical Constraints on the Symmetry Energy and the Neutron Skin of 208Pb with Minimal Modeling Assumptions. Submitted to *Physical Review C*. (LA-UR-21-21363)

Essick, R., P. Landry, A. Schwenk and I. Tews. Astrophysical Constraints on the Symmetry Energy and the Neutron Skin of 208-Pb with Minimal Modeling Assumptions. Submitted to *Physical Review Letters*. (LA-UR-21-20527)

Essick, R., P. Landry, I. Tews, S. Reddy and D. E. Holz. Direct Astrophysical Tests of Chiral Effective Field Theory. Submitted to *Physical Review C*. (LA-UR-20-22615)

*Lonardoni, D., I. Tews, S. Gandolfi and J. A. Carlson. Nuclear and neutron-star matter from local chiral interactions. 2020. *Physical Review Letters*. **2** (2): 022033. (LA-UR-19-32538 DOI: 10.1103/PhysRevResearch.2.022033)

Lonardoni, D. and I. Tews. Local chiral EFT potentials in nuclei and neutron matter: results and issues. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-22185 DOI: 10.22323/1.317.0100)

Pang, P. T., T. Dietrich, I. Tews and C. Van Den Broeck. Parameter estimation for strong phase transitions in supranuclear matter using gravitational-wave astronomy. Submitted to *Physical Review Research*. (LA-UR-20-24019)

*Piarulli, M. and I. Tews. Local Nucleon-Nucleon and Three-Nucleon Interactions Within Chiral Effective Field Theory. 2020. *Frontiers in Physics*. **7**: 245. (LA-UR-19-30461 DOI: 10.3389/fphy.2019.00245)

Schwenk, A. and I. Tews. Nukleare Zustandgleichung aus Gravitationswellenbeobachtungen (Nuclear equation of state from gravitational-wave observations). Submitted to *Physikjournal*. (LA-UR-21-20533)

Somasundaram, R., C. Drischler, I. Tews and J. Margueron. Constraints on the nuclear symmetry energy from asymmetric matter calculations with chiral e ffective eld theory. Submitted to *Physical Review C*. (LA-UR-20-26894)

*Tews, I. Quantum Monte Carlo Methods for Astrophysical Applications. 2020. *Frontiers in Physics*. **8**. (LA-UR-19-32577 DOI: 10.3389/fphy.2020.00153)

Tews, I. What can neutron stars reveal about the equation of state of dense matter?. *EPJ Web of Conferences*. **235**: 07002. (LA-UR-20-21735 DOI: 10.1051/epjconf/202023507002)

Tews, I., D. Lonardoni, K. Hebeler and L. Huth. Local chiral interactions up to next-to-next-to-leading order at larger cutoffs. Submitted to *Physical Review C*. (LA-UR-21-20525)

Tews, I., J. Margueron and S. Reddy. To which extend nuclear physics and GW170817 constrain the neutron star equation of state?. Submitted to *Proceedings for the CUSTIPEN XiAMEN Workshop*. (LA-UR-19-24461)

Tews, I., P. T. Pang, T. Dietrich, M. W. Coughlin, S. Antier, M. Bulla, J. Heinzel and L. Issa. On the Nature of GW190814 and Its Impact on the Understanding of Supranuclear

Matter. 2021. *The Astrophysical Journal Letters*. **908** (1). (LA-UR-20-24959 DOI: 10.3847/2041-8213/abdaae)

Tews, I., P. T. Pang, T. Dietrich, M. W. Coughlin and M. Bulla. Impact of new NICER data on the equation of state of nuclear matter. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-20534)

Tews, I., Z. Davoudi, A. Ekstrom, J. D. Holt and J. E. Lynn. New ideas in constraining nuclear forces. 2020. *Journal of Physics G: Nuclear and Particle Physics*. **47** (10): 103001. (LA-UR-19-32540 DOI: 10.1088/1361-6471/ab9079)

Reports

Dietrich, T. and I. Tews. Neutronensterne befl\xc3\xbcgeln Kosmologie und Kernphysik (Neutron stars spur cosmology and nuclear physics). *Spektrum der Wissenschaften (German popular science magazine)*. (LA-UR-21-20811)

Presentation Slides

Tews, I. Chiral effective field theory for the nuclear equation of state and neutron-star mergers. Presented at *2019 Fall Meeting of the APS Division of Nuclear Physics*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30581)

Tews, I. Chiral Effective Field Theory, Dense Nuclear Matter, and Neutron-Star Mergers. Presented at *JINA-INT Workshop Dense Matter & Neutron Star Mergers*, Seattle, Washington, United States, 2019-12-16 - 2019-12-18. (LA-UR-19-32539)

Tews, I. Stringent constraints on neutron-star radii from neutron-star mergers and chiral effective field theory. Presented at *Hirschegg 2020*, Hirschegg, Austria, 2020-01-13 - 2020-01-13. (LA-UR-20-20236)

Tews, I. Constraining the neutron-star equation of state and radius with chiral effective field theory and observations. Presented at *Ringberg conference*, Kreuth, Germany, 2020-01-13 - 2020-01-13. (LA-UR-20-20431)

Tews, I. From nuclei to neutron stars with local chiral interactions. Presented at *Theory Seminar at Washington University in St. Louis*, St. Louis, Missouri, United States, 2020-02-27 - 2020-02-27. (LA-UR-20-21840)

Tews, I. Constraining the neutron-star equation of state and radius with chiral effective field theory and observations. . (LA-UR-20-22616)

Tews, I. Constraining neutron-star matter with chiral effective field theory. Presented at *Second Nuclear and Particle Theory Meeting*, online, Missouri, United States, 2020-05-11 - 2020-05-12. (LA-UR-20-23507)

Tews, I. Nuclear-physics and multi-messenger constraints on the neutron-star equation of state. Presented at *Astrophysics/Gravity/Cosmology Seminar at University of Illinois at Urbana-Champaign (online)*, Los Alamos, New Mexico, United States, 2020-11-04 - 2020-11-04. (LA-UR-20-28940)

Tews, I. Dense-Matter Nuclear Theory. Presented at *JINA Horizons Virtual Meeting*, Los Alamos, New Mexico, United States, 2020-12-01 - 2020-12-04. (LA-UR-20-29793)

Tews, I. Nuclear-physics and multi-messenger constraints on the neutron-star equation of state. Presented at *IReNA online seminar*, Los Alamos, New Mexico, United States, 2020-12-11 - 2020-12-11. (LA-UR-20-30077)

Tews, I. NERSC Highlight slide. . (LA-UR-21-20568)

Tews, I. Quantum Monte Carlo Methods with chiral EFT Interactions as a consistent Approach to Nuclei and Neutron Stars. . (LA-UR-21-20814)

Tews, I. The nuclear equation of state in the era of neutron-star mergers. . (LA-UR-21-21910)

Posters

Tews, I. Matter and Nuclei at Neutron-rich Extremes. . (LA-UR-19-25831)

Tews, I. Neutron-Star Mergers as Probes for Nuclear Physics. Presented at *NUCLEI SciDAC PI meeting*, Rockville, Maryland, United States, 2019-07-15 - 2019-07-18. (LA-UR-19-26620)

State-of-the-Art Predictions for the Matter-Antimatter Asymmetry

Christopher Lee
20190622PRD2

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.

Publications

Journal Articles

Fuyuto, K., M. Ramsey-Musolf, C. Chiang, G. Cottin and Y. Du. Collider probes of real triplet scalar dark matter. 2021. *Journal of High Energy Physics*. **2021** (1): 198. (LA-UR-20-22358 DOI: 10.1007/JHEP01(2021)198)

Fuyuto, K., V. Cirigliano, C. Lee, E. Mereghetti and B. Yan. Charged lepton flavor violation at the EIC. Submitted to *Journal of High Energy Physics*. (LA-UR-21-20531)

*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 Letters*. **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)

Phase Diagrams and Conductivity in the Interiors of White Dwarf Stars

Didier Saumon
20190624PRD2

Project Description

The extreme conditions found in stars and the wide range of multi-physics problems that must be solved to understand them overlaps considerably with the science of national security at the Laboratory. Astrophysics is a field where advanced models can be developed and tested and then applied to national security challenges. White dwarf stars in particular present exotic physical conditions not found in any other type of star and pose challenging problems to solve. The proposed work will address the calculation of material properties that are difficult to model, in particular the melting of mixtures and heat transport. These are two essential components for the modeling of white dwarfs. Our accurate plasma models and calculations will lead to better white dwarf models, with consequences for several fields of astrophysics. Moreover, the methods and tools we will develop are more generally applicable to the melting of pure substances and alloys, as well as heat transport in systems such as inertial confinement fusion. We anticipate that they will find fruitful applications in several areas of high energy density physics of relevance to national security, such as stockpile stewardship, where accurate material properties are a critical element to our theoretical understanding.

Publications

Journal Articles

*Blouin, S. Magnesium abundances in cool metal-polluted white dwarfs. 2020. *Monthly Notices of the Royal Astronomical Society*. **496** (2): 1881-1890. (LA-UR-20-23364 DOI: 10.1093/mnras/staa1689)

*Blouin, S., J. Daligault, D. Saumon, A. Bedard and P. Brassard. Toward precision cosmochronology. 2020. *Astronomy & Astrophysics*. **640**: L11. (LA-UR-20-24795 DOI: 10.1051/0004-6361/202038879)

Blouin, S., J. O. Daligault and D. Saumon. 22Ne Phase Separation As A Solution To The Ultramassive White Dwarf Cooling Anomaly. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-22409)

*Blouin, S., N. R. Shaffer, D. Saumon and C. E. Starrett. New Conductive Opacities for White Dwarf Envelopes. 2020. *The Astrophysical Journal*. **899** (1): 46. (LA-UR-20-24054 DOI: 10.3847/1538-4357/ab9e75)

Blouin, S. and J. O. Daligault. Direct Evaluation of the Phase Diagrams of Dense Multicomponent Plasmas by Integration of the Clapeyron Equations. Submitted to *Physical Review E*. (LA-UR-21-20287)

*Blouin, S. and P. Dufour. The evolution of carbon-polluted white dwarfs at low effective temperatures. 2019. *Monthly Notices of the Royal Astronomical Society*. **490** (3): 4166-4174. (LA-UR-19-29175 DOI: 10.1093/mnras/stz2915)

Harrison, J., A. Bonsor, M. Kama, A. Buchan and S. Blouin. Bayesian constraints on the origin and geology of exo-planetary material using a population of externally polluted white dwarfs. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-20941)

Kaiser, B. C., J. C. Clemens, S. Blouin, P. Dufour, R. J. Hegedus, J. S. Reding and A. B\xc3\xa9dard. Exo-Planetesimal Lithium Pollution of a White Dwarf. Submitted to *Science*. (LA-UR-20-24419)

*Kilic, M., P. Bergeron, A. Kosakowski, W. R. Brown, M. A. Ag\xc3\xbceros and S. Blouin. The 100 pc White Dwarf Sample in the SDSS Footprint. 2020. *The Astrophysical Journal*. **898** (1): 84. (LA-UR-20-23514 DOI: 10.3847/1538-4357/ab9b8d)

Kilic, M., P. Bergeron, S. Blouin and A. B\xc3\xa9dard. The Most Massive White Dwarfs in the Solar Neighborhood. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-20639)

Klein, B., A. Doyle, B. Zuckerman, P. Dufour, S. Blouin, C. Melis, A. Weinberger and E. Young. Discovery of Beryllium in White Dwarfs Polluted by Accreted Planetesimals. Submitted to *Astrophysical Journal*. (LA-UR-20-29805)

*Klein, B., S. Blouin, D. Romani, B. Zuckerman, C. Melis, S. Xu, P. Dufour, C. Genest-Beaulieu, A. Bedard and M. Jura. Atmospheric Temperature Inversions and He i 5876 Core Profile Structure in White Dwarfs. 2020. *The Astrophysical Journal*. **900** (1): 2. (LA-UR-20-22642 DOI: 10.3847/1538-4357/ab9b24)

*Lam, M. C., N. C. Hambly, N. Lodieu, S. Blouin, E. J. Harvey, R. J. Smith, M. C. Galvez-Ortiz and Z. H. Zhang. First discovery of an ultra-cool white dwarf benchmark in common proper motion with an M dwarf. 2020. *Monthly Notices of the Royal Astronomical Society*. **493** (4): 6001-6010. (LA-UR-19-31660 DOI: 10.1093/mnras/staa584)

Vanderbosch, Z., S. Rappaport, J. A. Guidry, B. L. Gary, S. Blouin, T. G. Kaye, A. Weiberger, C. Melis, B. Klein, B. Zuckerman, A. Vanderburg, J. Hermes, R. J. Hegedus, M. R. Burleigh, R. Sefako and T. M. Heintz. ZTF J0328-1219: A Third Case of Transiting Planetary Debris around a White Dwarf. Submitted to *Astrophysical Journal*. (LA-UR-21-21884)

*Vanderburg, A., S. A. Rappaport, S. Xu, I. Crossfield, J. C. Becker, B. Gary, F. Murgas, S. Blouin and l. i. t. p. And 53 other non-LANL authors. A giant planet candidate transiting a white dwarf. 2020. *Nature*. **585** (7825): 363-367. (LA-UR-20-21720 DOI: 10.1038/s41586-020-2713-y)

Conference Papers

Blouin, S. and P. Dufour. The Spectral Evolution of Cool White Dwarfs. Presented at *IAU Symposium 357: White Dwarfs as probes of fundamental physics and tracers of planetary, stellar & galactic evolution*. (Hilo, Hawaii, United States, 2019-10-21 - 2019-10-25). (LA-UR-19-31433)

Presentation Slides

Blouin, S. The spectral evolution of cool white dwarfs. Presented at *International Astronomical Union Symposium 357: White Dwarfs as probes of fundamental physics and tracers of planetary, stellar & galactic evolution*, Hilo, Hawaii, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-29925)

Blouin, S. When The Fit Is Just Right: Improved Cool White Dwarf Atmosphere Models. Presented at *235th Meeting of the American Astronomical Society*, Honolulu, Hawaii, United States, 2020-01-04 - 2020-01-08. (LA-UR-19-32098)

Blouin, S. Cool white dwarf atmospheres: From condensed matter physics to stellar archeology. Presented at *Annual Meeting of the Canadian Astronomical Society*, Online meeting, Canada, 2020-05-25 - 2020-05-28. (LA-UR-20-23444)

Blouin, S. Cool white dwarf atmospheres: From condensed matter physics to stellar archeology. Presented at *Annual Meeting of the Canadian Astronomical Society*, Online meeting, Canada, 2020-05-25 - 2020-05-28. (LA-UR-20-23636)

Blouin, S. Cool white dwarf atmospheres: A transparent window into the past. Presented at *Space Telescope Science Institute Seminar (remote)*, Baltimore, Maryland, United States, 2020-09-03 - 2020-09-03. (LA-UR-20-26543)

Blouin, S. Cool white dwarf atmospheres: A transparent window into the past. Presented at *Space Telescope Science Institute Seminar (remote)*, Baltimore, Maryland, United States, 2020-09-03 - 2020-09-03. (LA-UR-20-27315)

Blouin, S. Calculating Melting Curves for Crystallizing Stars. Presented at *XCP Seminar*, Los Alamos, New Mexico, United States, 2020-11-05 - 2020-11-05. (LA-UR-20-28803)

Blouin, S., J. O. Daligault, N. R. Shaffer, D. Saumon, A. B \xc3\xa9dard, P. Brassard and C. E. Starrett. New Melting Curves and Conductive Opacities for White Dwarfs. Presented at *237th Meeting of the American Astronomical Society*, Online, New Mexico, United States, 2021-01-11 - 2021-01-15. (LA-UR-21-20081)

Blouin, S., J. O. Daligault and D. Saumon. A New C/O Plasma Melting Curve For White Dwarf Core Crystallization. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28917)

Searching for Dark Matter with Fixed Target Experiments

Daniele Spier Moreira Alves
20190626PRD2

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.

Publications

Journal Articles

deNiverville, P., A. Berlin, A. Ritz, N. Toro and P. Schuster. On sub-GeV Dark Matter Production at Fixed-Target Experiments. Submitted to *Physical Review D*. (LA-UR-20-22261)

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)

The Ultimate Search for the Color Glass Condensate

Ivan Vitev
20200683PRD1

Project Description

The internal structure and dynamics of protons, neutrons and nuclei is one of the greatest scientific puzzles of our time. The simple image of the proton as three quarks bound together by the strong interaction via exchange of gluons is rendered immensely complicated by the fact that gluons themselves interact with each other. Thus, the origin of the proton spin is still not known, nor do we yet understand the origin of its mass and the mass of visible matter. One of the big theoretical discoveries of the late 20th century is that at extremely high energies nucleons and nuclei that make up our universe exhibit remarkable simplicity and evolve into a dense saturated state of gluons. This new state of matter, known as the Color Glass Condensate (CGC), may hold the answers to those puzzles. The Electron-Ion Collider (EIC), the number one priority for a new facility for the US Department of Energy, will be a perfect microscope into the content of hadrons and the ideal machine to discover gluon saturation and revolutionize our understanding of matter at all length scales. This research will develop the tools needed to discover the Color Glass Condensate and enhance EIC science.

Publications

Books/Chapters

Lee, C., I. M. Vitev, R. Boussarie, J. W. Qiu, I. W. Stewart, T. Mehen, M. Burkardt, M. Constantinou, W. Detmold, M. Ebert, M. Engelhardt, S. Fleming, L. Gamberg, X. Ji, Z. B. Kang, K. F. Liu, S. Liuti, A. Metz, J. Negele, D. Pitonyak, A. Prokudin, A. Rajan, M. Schlegel, P. Shanahan, P. Schweitzer, A. Tarasov, R. Venugopalan, F. Yuan and Y. Zhao. TMD Handbook: A modern introduction to the physics of Transverse Momentum Dependent distributions. (LA-UR-21-20798)

A Study of Diffusion Around Pulsar Wind Nebulae

James Harding
20200684PRD2

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.

Publications

Journal Articles

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)

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)

Towards Data Science Driven Multi-physics Modeling to Probe Neutron Star Mergers

Jonah Miller
20200687PRD2

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 post-merger accretion disks. Submitted to *Astrophysical Journal*. (LA-UR-20-28607)

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)

Decipher the Coupled Plasma and Atomic Physics for Reactor Plasma Exhaust

Xianzhu Tang
20200753PRD3

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.

Dark Matter and the Validity of Effective Field Theories

Jessica Goodman
20170661PRD1

Project Description

Discovering and understanding the physics of dark matter is a high priority in high-energy physics. This project will develop new theoretical models of dark matter and confront those against a variety high-energy physics experimental data. This project will develop simplified models for new dark matter physics scenarios in which interactions with Standard Model particles are generated at the quantum (i.e., loop) level. The current and projected sensitivity of the Large Hadron Collider (LHC) experiment to such scenarios will be assessed.

Technical Outcomes

This project began by systematically considering completions of effective operators which couple dark matter (DM) to the Standard Model via loop processes. The team wrote down a Lagrangian to describe the DM-mediator and mediator-SM interactions and calculated the DM production cross section at the parton level "by-hand."

First Principles Approach to Factorization Violation

Duff Neill
20170662PRD1

Project Description

This project advances our understanding of the quantum behavior of the most fundamental building blocks of matter that we know about, protons and the quarks and gluons that they are made of. The project will produce a quantitative theoretical framework to predict the effects of low-energy, long-wavelength gluon radiation between protons as they collide. Such proton collisions are the primary window we have into the nature of their constituents and the fundamental strong force between them. Discoveries of new particles, new forces, and the quantum laws of nature they reveal have underpinned some of the most revolutionary technological advances in the 20th, and now 21st, century. The DOE Office of Science, through the Offices of High-Energy and Nuclear Physics, supports major proton collider experiments in the US such as at the Fermilab accelerator in Illinois and the Relativistic Heavy-Ion Collider at Brookhaven in New York. This project will improve our ability to interpret the results of proton collision experiments at these facilities in terms of the underlying physics. These experiments and theory efforts to support them are highlighted in the National Nuclear Science Advisory Committee's 2015 Long-Range Plan as among the highest scientific priorities in the US.

Technical Outcomes

This project created an improved understanding and technical tools in how to calculate factorization violating effects and their connection to similar problems encountered in jet physics, relevant for the Department of Energy (DOE) efforts at the Large Hadron Collider and the up-coming Electron Ion Collider to understand the fundamental structure of nucleons.

Publications

Journal Articles

*Bertolini, D., D. Kolodrubetz, D. Neill, P. Pietrulewicz, I. W. Stewart, F. J. Tackmann and W. J. Waalewijn. Soft functions for generic jet algorithms and observables at hadron colliders. 2017. *Journal of High Energy Physics*. **2017** (7): 99. (LA-UR-17-23006 DOI: 10.1007/JHEP07(2017)099)

*Cal, P., D. Neill, F. Ringer and W. J. Waalewijn. Calculating the angle between jet axes. 2020. *Journal of High Energy Physics*. **2020** (4): 211. (LA-UR-19-31533 DOI: 10.1007/JHEP04(2020)211)

*Larkoski, A. J., I. Moult and D. Neill. Factorization and resummation for groomed multi-prong jet shapes. 2018. *Journal of High Energy Physics*. **2018** (2): 144. (LA-UR-17-29531 DOI: 10.1007/JHEP02(2018)144)

*Neill, D. A., Z. B. Kang, F. Ringer, K. Lee and X. Liu. The soft drop groomed jet radius at NLL. 2020. *Journal of High Energy Physics*. **2020** (2): 54. (LA-UR-19-30463 DOI: 10.1007/JHEP02(2020)054)

*Neill, D., A. Papaefstathiou, W. J. Waalewijn and L. Zoppi. Phenomenology with a recoil-free jet axis: TMD fragmentation and the jet shape. 2019. *Journal of High Energy Physics*. **2019** (1): 67. (LA-UR-18-30361 DOI: 10.1007/JHEP01(2019)067)

*Neill, D. and F. Ringer. Soft fragmentation on the celestial sphere. 2020. *Journal of High Energy Physics*. **2020** (6): 86. (LA-UR-20-21841 DOI: 10.1007/JHEP06(2020)086)

*Neill, D. and W. J. Waalewijn. Entropy of a Jet. 2019. *Physical Review Letters*. **123** (14): 142001. (LA-UR-18-30360 DOI: 10.1103/PhysRevLett.123.142001)

Jets in Strongly Interacting Plasmas

Andrey Sadofyev
20170666PRD1

Project Description

The Quark-Gluon Plasma (QGP) is a novel state of matter recently discovered in experiments at the Relativistic Heavy-Ion Collider (RHIC) at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research, CERN (from the French Conseil Européen pour la Recherche Nucléaire). An extremely dense and hot “fireball” is created in collisions of heavy ions and consists of the elementary constituents of matter, quark, and gluons, otherwise confined into protons and neutrons. It is also subject to the highest known magnetic field in the Universe, giving unique opportunity to study properties of plasmas at these extreme conditions. This research will result in a novel theoretical tool for studying the microscopic properties of strongly interacting matter. It will not only shed light on the phenomena that govern the QGP behavior, but also give insight into system such as the plasmas in the early universe, high-temperature superconductors, and unitary cold atoms. The work will pave the way to implementing modern theoretical methods and will provide guidance for the experimental study of QGP. It also will give valuable insights into energy loss of charged particles and plasma excitations in other extreme environments, relevant to national security applications.

Technical Outcomes

This project successfully developed a novel description of the jet-medium interaction in heavy-ion collisions, which can consistently include effects driven by physics at different length scales. This description is based on a hybrid holographic approach which had been applied to qualitative and quantitative studies of jet observables in heavy-ion experiments. The project also studied the transport properties of the quark-gluon plasma, particularly focusing on its anomalous dynamics.

Publications

Journal Articles

*Avdoshkin, A., A. V. Sadofyev and V. I. Zakharov. IR properties of chiral effects in pionic matter. 2018. *Physical Review D*. **97** (8): 085020. (LA-UR-17-31504 DOI: 10.1103/PhysRevD.97.085020)

*Brewer, J., K. Rajagopal, A. Sadofyev and W. van der Schee. Evolution of the mean jet shape and dijet asymmetry distribution of an ensemble of holographic jets in strongly coupled plasma. 2018. *Journal of High Energy Physics*. **2018** (2): 15. (LA-UR-17-29843 DOI: 10.1007/JHEP02(2018)015)

*Hirono, Y., D. E. Kharzeev and A. V. Sadofyev. Dynamics of Vortices in Chiral Media: The Chiral Propulsion Effect. 2018. *Physical Review Letters*. **121** (14): 142301. (LA-UR-18-22126 DOI: 10.1103/PhysRevLett.121.142301)

*Huang, X. and A. V. Sadofyev. Chiral vortical effect for an arbitrary spin. 2019. *Journal of High Energy Physics*. **2019** (3): 84. (LA-UR-18-24524 DOI: 10.1007/JHEP03(2019)084)

*Reiten, J. and A. V. Sadofyev. Drag force to all orders in gradients. 2020. *Journal of High Energy Physics*. **2020** (7): 146. (LA-UR-20-20237 DOI: 10.1007/JHEP07(2020)146)

Sadofyev, A., P. Mitkin, E. Speranza and X. Huang. Zilch Vortical Effect, Berry Phase, and Kinetic Theory. Submitted to *Journal of High Energy Physics*. (LA-UR-20-25498)

Sadofyev, A., W. van der Schee and J. Brewer. Jet shape modifications in holographic dijet systems. Submitted to *Physical Review Letters*. (LA-UR-18-30400)

Sadofyev, A. and E. Mottola. Chiral Waves on the Fermi-Dirac Sea: Quantum Superfluidity and the Axial Anomaly. Submitted to *Physical Review D*. (LA-UR-19-27117)

*Sadofyev, A. and S. Sen. Chiral anomalous dispersion. 2018. *Journal of High Energy Physics*. **2018** (2): 99. (LA-UR-17-31502 DOI: 10.1007/JHEP02(2018)099)

Shock-accelerated Variable-density Mixing in a Subsonic Cross Flow

Katherine Prestridge
20180714PRD2

Project Description

Accurate predictive simulations of turbulent mixing require experimental data under the relevant flow conditions, because our computation capability requires us to model the smallest scales of mixing-we do not have the capability to simulate all of the important length scales of realistic flows. The Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) are interested in shock-driven mixing with strong density gradients. This experimental facility and its diagnostics are designed to measure flows in regimes of interest, and the data are used to make improvements to models. The data improve our code capabilities. In addition to the technical outcomes, this facility and team provides training to new scientists on diagnostics for experiments, data analysis techniques, and collaborations among experiments, modelers, and numerical physicists.

Technical Outcomes

A novel experimental campaign provided insight into how gases are mixed together by shock waves. Because of the careful control of the initial conditions between the two gases before they were shocked, a new empirical rational function was discovered that predicts how much the gases will mix after the passage of the shock. This has implications for understanding how turbulent mixing impedes fusion in Inertial confinement fusion (ICF) capsules, and how supernova explosions generate elements in the universe.

Publications

Journal Articles

Mansoor, M. M., S. M. Dalton, A. A. Martinez, T. Desjardins, J. J. Charonko and K. P. Prestridge. The effect of initial conditions on mixing transition of the Richtmyer–Meshkov instability. 2020. *Journal of Fluid Mechanics*. **904**: A3. (LA-UR-19-31658 DOI: 10.1017/jfm.2020.620)

Conference Papers

Mansoor, M. M., S. M. Dalton, T. Desjardins, A. A. Martinez, J. J. Charonko and K. P. Prestridge. THE EFFECT OF INITIAL CONDITIONS ON THE LATE-TIME DEVELOPMENT OF RICHTMYER-MESHKOV INSTABILITY. Presented at *Eleventh International Symposium on Turbulence and Shear Flow Phenomena (TSFP11)*. (Southampton, United Kingdom, 2019-07-30 - 2019-08-02). (LA-UR-19-23718)

Presentation Slides

Prestridge, K. P., M. M. Mansoor, A. A. Martinez, S. M. Dalton and T. Desjardins. Effects of initial conditions on shock-driven instabilities and turbulent mixing. Presented at *Eleventh International Symposium on Turbulence and Shear Flow Phenomena (TSFP11)*, Southampton, United Kingdom, 2019-07-30 - 2019-08-02. (LA-UR-19-27196)

Posters

Mansoor, M. M., S. M. Dalton, J. J. Charonko, A. A. Martinez and K. P. Prestridge. Vortex Ejections in Converging Jets. Presented at *American Physical Society Division of Fluid dynamics*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-29891)

Martinez, A. A., J. J. Charonko, M. M. Mansoor, S. M. Dalton and K. P. Prestridge. Shock-driven mixing and turbulence. Presented at *Annual Meeting of the Division of Fluid Dynamics*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-30620)

Extreme Radiation Magnetohydrodynamics Around Black Holes

Benjamin Ryan
20180716PRD2

Project Description

The primary goal of the research is to better understand physical phenomena that occur under the extreme conditions near black holes. In pursuing this goal, expertise and numerical techniques for a range of physical processes of relevance to DOE/NNSA missions will be developed. The expected outcomes include multiple impactful publications and a well-trained early career scientist that will be well-positioned to contribute to Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions in the long term.

Technical Outcomes

This project both developed novel numerical methods for radiation magnetohydrodynamics, and applied those methods to accreting black holes. In pursuing this goal, expertise and numerical techniques relevant to the Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions were developed. This project both leveraged an existing method we developed to interpret the Event Horizon Telescope imaging of M87 that was recognized by the 2020 Breakthrough Prize in Fundamental Physics, as well as developed a novel radiation hydrodynamics method, Method of Characteristics Moment Closure.

Publications

Journal Articles

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Ryan, B. R. and J. C. Dolence. MOCMC: Method of Characteristics Moment Closure, a Numerical Method for Covariant Radiation Magnetohydrodynamics. Submitted to *Astrophysical Journal. Supplement Series*. (LA-UR-19-24802)

Presentation Slides

Dolence, J. C. Full Transport GR Neutrino Radiation MHD and Nucleosynthesis in Neutron Star Merger Disks. Presented at *Explosive Nucleosynthesis in the Supernova and Merging-Neutron-Star Contexts*, Princeton, New Jersey, United States, 2019-05-22 - 2019-05-24. (LA-UR-19-24793)

Ryan, B. R. MOCMC Status Report & Rad Hydro Issues. Presented at *TCAN 2020*, New York, New York, United States, 2020-01-09 - 2020-01-11. (LA-UR-20-20323)

Ryan, B. R. w19_ebhlight3d: 3D Radiation Magnetohydrodynamic Simulations of Accreting Black Holes. . (LA-UR-20-26965)

Ryan, B. R. and J. C. Dolence. Method of Characteristics Moment Closure, a Numerical Method for Covariant Radiation Magnetohydrodynamic. Presented at *The 26th International Conference on Transport Theory (ICTT-26)*, Paris, France, 2019-09-23 - 2019-09-27. (LA-UR-19-29627)

Ryan, B. R. and J. C. Dolence. METHOD OF CHARACTERISTICS MONTE CARLO. Presented at *Horizon Collaboration Meeting 2019*, Princeton, New Jersey, United States, 2019-04-14 - 2019-04-16. (LA-UR-19-23499)

Unraveling Nature's Mysteries at the World's Highest Energy Colliders

Ivan Vitev
20180748PRD3

Project Description

Showers of subatomic particles, called jets, are ubiquitous in nature. For example, cosmic jets are a cornerstone of modern astrophysics and collimated beams of electrons and photons find applications ranging from material science to nuclear medicine. However, nowhere are jets of elementary particles more copiously produced and comprehensively studied than at the modern high energy and nuclear physics collider facilities. This project will develop state of the art theory of jets to interpret experimental data, understand the origin of mass, and unravel the properties of extremely hot and dense state of matter in the early universe. Similar systems are also of interest to national security physics applications.

Technical Outcomes

This project significantly advanced the theory of jets of elementary particles most copiously produced at modern high energy and nuclear physics collider facilities. Specifically, the team developed new effective theories to describe jets that contain heavy subatomic particles, understood the flow of energy inside jets, and provided the most accurate calculations of the shape of high-energy collision events. The team also advanced the understanding of the recently discovered Higgs particle.

Publications

Journal Articles

*Chen, L., H. T. Li, H. Shao and J. Wang. Higgs boson pair production via gluon fusion at N3LO in QCD. 2020. *Physical Review Letters*. **803**: 135292. (LA-UR-19-30443 DOI: 10.1016/j.physletb.2020.135292)

*Chen, L., H. T. Li, H. Shao and J. Wang. The gluon-fusion production of Higgs boson pair: N3LO QCD corrections and top-quark mass effects. 2020. *Journal of High Energy Physics*. **2020** (3): 72. (LA-UR-20-20034 DOI: 10.1007/JHEP03(2020)072)

*Gao, A., H. T. Li, I. Moult and H. X. Zhu. Precision QCD Event Shapes at Hadron Colliders: The Transverse Energy-Energy Correlator in the Back-to-Back Limit. 2019. *Physical Review Letters*. **123** (6): 062001. (LA-UR-19-20914 DOI: 10.1103/PhysRevLett.123.062001)

*Li, C. S., H. T. Li, D. Y. Shao and J. Wang. Momentum-space threshold resummation in tW production at the LHC. 2019. *Journal of High Energy Physics*. **2019** (6): 125. (LA-UR-19-21475 DOI: 10.1007/JHEP06(2019)125)

Li, H. T. and I. Vitev. Jet splitting function in the vacuum and QCD medium. *PoS - Proceedings of Science*. (LA-UR-19-20679 DOI: 10.22323/1.345.0077)

*Li, H. T. and I. Vitev. Inclusive heavy flavor jet production with semi-inclusive jet functions: from proton to heavy-ion collisions. 2019. *Journal of High Energy Physics*. **2019** (7): 148. (LA-UR-19-20952 DOI: 10.1007/JHEP07(2019)148)

Li, H., I. M. Vitev and Y. J. Zhu. Transverse-Energy-Energy Correlations in Deep Inelastic Scattering. Submitted to *Journal of High Energy Physics*. (LA-UR-20-24408)

*Li, H. and I. M. Vitev. Jet charge modification in finite QCD matter. 2020. *Physical Review D*. **101** (7): 076020. (LA-UR-19-30442 DOI: 10.1103/PhysRevD.101.076020)

Conference Papers

Li, H. Jet charge in heavy-ion collisions. Presented at *https://indico.cern.ch/event/761800/*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-09). (LA-UR-20-21864)

Modeling Late-Time Electromagnetic Pulse and Its Disturbed Atmospheric Environment

Christopher Jeffery
20190541MFR

Project Description

A high-altitude nuclear explosion (HANE) can significantly disturb the Earth's upper atmosphere, resulting in the generation of a late-time electromagnetic pulse (EMP) and an environment that negatively affects radio wave propagation across a broad range of frequencies. We are developing a computer model that will allow us to simulate the disturbance of the atmosphere by a HANE, the generation of EMP in this disturbed atmosphere, and the subsequent development of an environment that could greatly impair the efficacy of radio communications.

Publications

Reports

M. Jeffery, C. A. Introducing GeoRad: A Variable-Resolution EMP Solver on an Unstructured Voronoi Tessellation. Unpublished report. (LA-UR-19-29953)

Presentation Slides

M. Jeffery, C. A., E. H. Lay, K. R. Costigan, W. P. Even, E. M. Nelson, H. E. Morris and M. J. Peterson. The Nuclear-Disturbed Environment: E3, HF/VHF Absorption & the Monitoring Potential of Our SNDD EMP System. Presented at *SGSIE 2020*, Los Alamos, New Mexico, United States, 2020-11-02 - 2020-11-06. (LA-CP-20-20658)

Posters

M. Jeffery, C. A., E. H. Lay, K. R. Costigan, W. P. Even, H. E. Morris and M. Worstell. Modeling High-Energy Disturbances in GeoRad: Impacts on D-Region Chemistry and Knapp's Three Species Model. Presented at *Fall AGU*, Online, New Mexico, United States, 2020-12-15 - 2020-12-15. (LA-UR-20-30243)

M. Jeffery, C. A., K. R. Costigan, E. H. Lay and H. E. Morris. Test of a Multigrid Method for Ionospheric Temperature Modeling. Presented at *Fall AGU*, San Francisco, California, United States, 2019-12-13 - 2019-12-13. (LA-UR-19-32621)

Superconducting Radio-frequency (SRF) Cavities: Looking Beyond Niobium

Evgenya Simakov
20200439MFR

Project Description

This project offers an innovative approach towards lowering the surface resistance of superconducting radio-frequency (SRF) accelerating structures for high gradient proton and electron accelerators. SRF cavities are now regularly produced to operate very close to the fundamental limits of niobium. However, gradients achievable in SRF cavities are still limited. At Los Alamos, we have developed a unique method which may allow us to coat internal surface of the SRF structures with niobium-germanium (Nb3Ge), which is a superior superconducting material. This project will provide cost-effective solutions for future Los Alamos Neutron Science Center (LANSCE) modernizations and upgrade to 3 giga-electron volt (GeV) proton radiography (pRad), as well as reduce the cost of the planned Dynamic Mesoscale Material Science Capability (DMMSC) project.

Technical Outcomes

This project developed a unique method for coating the internal surface of superconducting radio-frequency (SRF) structures with niobium-germanium (Nb3Ge), which is a superior superconducting material. This project demonstrated niobium-germanium (Nb3Ge) films on small coupons with correct stoichiometry. This project also produced niobium-tin (Nb3Sn) films on various substrates that demonstrated superconducting transitions at temperatures ranging from 7 Kelvin (K) to 16.5K. Importantly, one sample of Nb3Sn coated on Nb substrate and annealed at a relatively low temperature of 700 celsius demonstrated the transition temperature of 14.5K. Results from this project suggest feasibility of using the Los Alamos sputtering method for producing Nb3Sn coatings on materials other than Nb, such as copper.

Publications

Posters

Simakov, E. I. and I. O. Usov. SRF Cavities: looking beyond niobium. Presented at *2020 Engineering Capability Review*, LOS ALAMOS, New Mexico, United States, 2020-09-09 - 2020-09-09. (LA-UR-20-26711)

Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors

Holly Trellue
20190649DI

Project Description

Innovative nuclear reactor designs are currently being proposed to increase efficiency and economic viability of nuclear energy production. Microreactors are one example of a portable reactor concept that can provide power in remote environments. In support of these designs, moderated materials such as yttrium hydride provide reductions in the size requirements of the system. Understanding of hydrogen dynamics, i.e. the behavior of hydrogen atoms in materials as a function of temperature and hydrogen concentration, is of paramount importance for applications that assess material behavior (e.g. corrosion) of these advanced moderators. The combination of experimental results and advanced multi-physics simulation tools from this project will further our understanding and ultimately provide predictive capabilities of hydrogen behavior in a nuclear reactor. These capabilities can be applied to other hydrogen-related problems after the end of this project. A high fidelity hydrogen mapping capability will be developed at LANSCE, and a new multi-physics framework for a range of reactor design analysis will be generated.

Publications

Journal Articles

Mehta, V. K., J. C. Armstrong, V. R. Dasari and D. Kotlyar. Capturing Multiphysics Effects in Hydride Moderated Microreactors using MCNP and ABAQUS. Submitted to *Applied Sciences*. (LA-UR-21-20451)

Mehta, V. K., S. C. Vogel, A. P. Shivprasad, E. P. Luther, A. D. R. Andersson, V. R. Dasari, D. Kotlyar, M. W. D. Cooper and B. Clausen. A Density Functional Theory and Neutron Diffraction Study of the Ambient Condition Properties of Sub-Stoichiometric Yttrium Hydride. 2021. *Journal of Nuclear Materials*. 152837. (LA-UR-20-24029 DOI: 10.1016/j.jnucmat.2021.152837)

Mehta, V. K., S. C. Vogel, M. W. D. Cooper and D. Kotlyar. Direct Observation of Bredig Transition in Yttrium Hydride (YH2-x). Submitted to *Physical Review Letters*. (LA-UR-20-26447)

Mehta, V. K., S. C. Vogel, R. B. Wilkerson, D. Kotlyar, M. W. D. Cooper and V. R. Dasari. Evaluation of Yttrium Hydride (\xce\xb4-YH2-x) Thermal Neutron Scattering Laws and Thermophysical Properties. Submitted to *Nuclear Science and Engineering*. (LA-UR-20-26691)

Shivprasad, A. P., S. C. Vogel, V. K. Mehta, M. W. D. Cooper, T. A. Saleh, J. T. White, J. R. Wermer, E. P. Luther and H. R. Trellue. Thermophysical properties of high-density, sintered monoliths of yttrium dihydride in the range 373–773\xc2\xa0K. 2021. *Journal of Alloys and Compounds*. **850**: 156303. (LA-UR-20-23935 DOI: 10.1016/j.jallcom.2020.156303)

Conference Papers

Wilkerson, R. B., G. W. Mckinney, C. J. Josey, M. e. Blood, J. D. Galloway, J. C. Armstrong and H. R. Trellue. Advances in MCNP for Reactor Calculations. Presented at *American Nuclear Society Annual Meeting*. (Phoenix, Arizona, United States, 2020-06-07 - 2020-06-11). (LA-UR-20-20505)

Reports

Armstrong, J. C. and K. C. Kelley. Generating MCNP Input Files for Unstructured Mesh Geometries. Unpublished report. (LA-UR-20-27139)

Mehta, V. K. Investigating the Response of Yttrium Hydride Moderator Due to Changes in Stoichiometry and Temperature. Unpublished report. (LA-UR-20-23082)

Mehta, V. K. INVESTIGATING THE RESPONSE OF YTTRIUM HYDRIDE MODERATOR DUE TO CHANGES IN STOICHIOMETRY AND TEMPERATURE. Unpublished report. (LA-UR-20-29128)

Mehta, V. K. and J. C. Armstrong. Processing MCNP Elemental Edit Outputs. Unpublished report. (LA-UR-20-24025)

Wilkerson, R. B., G. McKinney, M. E. Rising and J. A. Kulesza. MCNP Reactor Multigroup Tally Options Verification. Unpublished report. (LA-UR-20-27819)

Presentation Slides

Armstrong, J. C. and M. E. Rising. MCNP Code Modernization & Code Improvement for Microreactor Multiphysics Calculations. . (LA-UR-20-23568)

Shivprasad, A. P., D. M. Frazer, E. P. Luther, S. C. Vogel, A. M. Long, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer, H. R. Trellue and V. R. Dasari. Properties of sintered yttrium dihydride for nuclear reactor moderator applications. Presented at *INTERNATIONAL CONFERENCE ON PROCESSING & MANUFACTURING OF ADVANCED MATERIALS (THERMEC 2021)*, Online, New Mexico, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-21862)

Shivprasad, A. P., E. P. Luther, A. M. Long, T. E. Cutler, T. J. Grove, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer and H. R. Trellue. High temperature moderator material for Microreactors. . (LA-UR-20-21710)

Shivprasad, A. P., E. P. Luther, S. C. Vogel, A. M. Long, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer, H. R. Trellue and V. R. Dasari. Thermophysical properties of sintered yttrium dihydride. Presented at *MS&T 2020*, Online, New Mexico, United States, 2020-11-02 - 2020-11-02. (LA-UR-20-28532)

Shivprasad, A. P., E. P. Luther, S. C. Vogel, T. E. Cutler, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer, H. R. Trellue and A. M. Long. High temperature moderator capabilities at LANL. Presented at *NASA Moderator TIM*, Los Alamos, New Mexico, United States, 2020-10-15 - 2020-10-15. (LA-UR-20-28214)

Shivprasad, A. P., V. K. Mehta, M. W. D. Cooper, T. A. Saleh, J. T. White, J. R. Wermer, E. P. Luther and H. R. Trellue. Thermophysical properties of yttrium dihydride. Presented at *44th International Conference and Expo on Advanced Ceramics and Composites (ICACC 2020)*, Daytona Beach, Florida, United States, 2020-01-26 - 2020-01-26. (LA-UR-20-20540)

Trellue, H. R., S. C. Vogel, A. M. Long, J. C. Armstrong, V. K. Mehta, M. W. D. Cooper, A. P. Shivprasad, E. P. Luther and M. e. Blood. Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors - FY19. . (LA-UR-19-30226)

Trellue, H. R., S. C. Vogel, A. M. Long, V. K. Mehta, J. C. Armstrong, G. W. Mckinney, A. P. Shivprasad, E. P. Luther, J. E. Payne, M. W. D. Cooper, D. T. Carver, R. B. Wilkerson, J. R. Wermer and J. S. Bull. Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors. . (LA-UR-20-22974)

Other

Mehta, V. K. Releasing Yttrium Hydride Thermal Scattering Laws (TSLs) for Cross Section Evaluation Working Group (CSEWG) peer review. Dataset. (LA-UR-21-21948)

Nuclear Material Control and Accounting (NMC&A)/In-line Monitoring Capability (DYnamic MAterials Control, DYMAC)

Rollin Lakis
20200668DI

Project Description

The primary goal of the DYnamic MAterials Control (DYMAC) Director's Initiative is to enhance The Los Alamos Plutonium Facility's (PF-4) manufacturing agility and efficiency, and improve nuclear security by modernizing, streamlining and optimizing quantitative nuclear material measurements and nuclear material control and accounting (NMC&A). Longer special nuclear material (SNM) inventory cycles and increased regulator 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 PF-4.

Adaptive Machine Learning for Advanced Diagnostics and Autonomous Control of Particle Accelerators

Alexander Scheinker
20200410DI

Project Description

The Department of Energy (DOE) utilizes some of the world's most advanced particle accelerators for research and development, just two examples are: 1). The Los Alamos Neutron Science Center provides intense neutron beams for basic material science research and basic science research, for the Weapons Neutron Research (WNR) Facility, which provides neutron and proton beams, and detector arrays for basic, applied, industrial, and defense-related research, and intense proton beams for dynamic experiments in support of national and international weapons science and stockpile stewardship programs via proton radiography. 2). The Linac Coherent Light Source Free Electron Laser provides extremely bright and short X-ray pulses for studying everything from biological processes to shock waves in materials relevant to DOE programs. The goals of this work are to improve such facilities by providing faster, more automated and more optimal tune up and operation, thereby providing more beam time and higher quality beams to all users, as well as to develop new capabilities, such as non-invasive diagnostics and more complex adaptive machine learning-based algorithms which can provide higher quality beams than is currently achievable and thereby enable future DOE facilities such as the Matter-Radiation Interactions in Extremes (MaRIE) facility.

Technical Outcomes

Adaptive feedback algorithms were developed and experiments on subsystems of the Los Alamos Neutron Science Center (LANSCE) accelerator were carried out proving the feasibility of our approach, a first step towards working with larger parameter sets and incorporating machine learning (ML) for a global adaptive ML control system. The development of a general machine learning framework for enforcing physics-based constraints has also begun and tested on several simulation-based problems.

Publications

Journal Articles

*Scheinker, A., S. Gessner, C. Emma and A. L. Edelen. Adaptive model tuning studies for non-invasive diagnostics and feedback control of plasma wakefield acceleration at FACET-II. 2020. *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. **967**: 163902. (LA-UR-20-23588 DOI: 10.1016/j.nima.2020.163902)

Conference Papers

Scheinker, A. Adaptive Feedback and Machine Learning for Particle Accelerators. Presented at *2020 International Particle Accelerator Conference*. (Ganil, France, 2020-05-10 - 2020-05-15). (LA-UR-20-23915)

Scheinker, A., P. H. Naffziger and A. R. Garcia. Extremum Seeking for Minimization of Beam Loss in the LANSCE Linear Accelerator by Tuning RF Cavities. Presented at *2020 American Control Conference*. (Denver, Colorado, United States, 2020-07-01 - 2020-07-03). (LA-UR-20-23916)

Scheinker, A. and D. Scheinker. Extremum Seeking for Creating Optimal Feedback Controls of Unknown Systems by Tuning Basis Functions. Presented at *2020 American Control Conference*. (Denver, Colorado, United States, 2020-07-01 - 2020-07-03). (LA-UR-20-23917)

Scheinker, A. and S. Gessner. Adaptive Machine Learning for Time Varying Systems: Noninvasive Diagnostics and Automatic Control for Short Intense Bunches. Presented at *Snowmass 2020*. (Batavia, Illinois, United States, 2020-11-04 - 2020-11-04). (LA-UR-20-26465)

Presentation Slides

Scheinker, A. Adaptive Feedback and Machine Learning for Particle Accelerators. Presented at *2020 International Particle Accelerator Conference*, Caen, France, 2020-05-11 - 2020-05-11. (LA-UR-20-23914)

Posters

Scheinker, A. MACHINE LEARNING FOR PARTICLE ACCELERATORS. Presented at *LANL engineering capabilities review*, Los Alamos, New Mexico, United States, 2020-09-21 - 2020-09-21. (LA-UR-20-26409)

Science of Signatures

Atomtronics: A New Approach to Sensing, Signal Processing, and Signal Analysis

Malcolm Boshier
20180045DR

Project Description

The project addresses three challenges facing the intelligence and defense communities: navigation when global position system (GPS) is unavailable or denied, unscrambling mixtures of radio signals received by multiple antennas (Blind Source Separation, or BSS), and determining the security of cryptography systems that rely on the presumed hardness of finding the prime factors of a large number. Our proposed solutions are based on atomtronics, the emerging science of circuits created from atoms flowing inside guides. We expect to demonstrate a compact atomtronic rotation sensor that outperfroms all existing technologies and therefore improves the accuracy of inertial navigation. We plan to build a prototype atomtronic signal processing circuit that can perform BSS. Finally, we will build an atomtronic device that finds the prime factors of numbers larger than any factored to date on quantum computers.

Publications

Journal Articles

Kim, H., K. A. Krzyzanowska, C. Ryu, K. C. Henderson, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple-loop atom interferometer. Submitted to *arXiv.org*. (LA-UR-20-28166)

*Ryu, C., E. C. Samson and M. G. Boshier. Quantum interference of currents in an atomtronic SQUID. 2020. *Nature Communications*. **11** (1): 3338. (LA-UR-20-25170 DOI: 10.1038/s41467-020-17185-6)

Presentation Slides

Boshier, M. G. DOE HEP and Quantum Sensing Research at Los Alamos National Laboratory. Presented at *Argonne Workshop on Quantum Sensing*, Chicago, Illinois, United States, 2017-12-12 - 2017-12-12. (LA-UR-17-31155)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31463)

Boshier, M. G. Two Experiments in Atomtronics: Quantum Interference in an Atomtronic SQUID and a Waveguide Sagnac Atom Interferometer. Presented at *2019 Benasque Atomtronics Workshop*, Benasque, Spain, 2019-05-05 - 2019-05-17. (LA-UR-19-24576)

Boshier, M. G. Lessons Learned From Developing Quantum Sensors. Presented at *STEP Workshop on Quantum Sensors*, McLean, Virginia, United States, 2019-09-10 - 2019-09-10. (LA-UR-19-29036)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *Quantum Technologies and Sensing Workshop*, Manchester, United Kingdom, 2019-10-27 - 2019-10-27. (LA-UR-19-30772)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *Seminar at Purdue University*, West Lafayette, Indiana, United States, 2019-11-12 - 2019-11-12. (LA-UR-19-31593)

Boshier, M. G. A Moving Waveguide Sagnac Atom Interferometer. Presented at *Workshop on Inertial Sensing*, Brighton, United Kingdom, 2019-11-29 - 2019-11-29. (LA-UR-19-32050)

Boshier, M. G., C. Ryu and C. Samson. Quantum \xc2\xa0Interference\xc2\xa0in\xc2\xa0an \xc2\xa0Atomtronic\xc2\xa0SQUID. Presented at *PQE-2018*, Snowbird, Utah, United States, 2018-01-08 - 2018-01-12. (LA-UR-18-20219)

Boshier, M. G. and C. Ryu. Atomtronics for Quantum Sensing. Presented at *2018 CINT User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-29086)

Henderson, K. C. Symmetry and How it Breaks. Presented at *New Mexico History Museum*, Santa Fe, New Mexico, United States, 2019-02-22 - 2019-02-22. (LA-UR-19-21059)

Kim, H. Detailed balance of thermalization dynamics in Rydberg quantum simulators. Presented at *LANL Quantum DAY*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31537)

Kim, H. Waveguide atom interferometer at LANL. . (LA-UR-21-22793)

Kurkcuoglu, D. M. Quantum simulation and quantum technologies with cold atoms. . (LA-UR-20-22384)

Martin, M. J., C. Ryu and M. G. Boshier. Quantum technologies with ultracold atoms. Presented at *UC Quantum Information Science Research Workshop*, Berkeley,

California, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24127)

Posters

Boshier, M. G. and C. Ryu. Sensing with Atomtronics Circuits and Devices. Presented at *SOS capability review*, Los Alamos, New Mexico, United States, 2018-04-24 - 2018-04-25. (LA-UR-18-23422)

Cassidy, M. C. Presentation2. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27193)

Hurd, S. J. Optimum Transportation of Cold Atoms. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27140)

Hurd, S. J. symposium poster sara hurd 2019. Presented at *Student Symposium*, Las Alamos, New Mexico, United States, 2019-08-07 - 2019-08-07. (LA-UR-19-27933)

Kim, H., J. Ferreras Fuertes, K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu and M. G. Boshier. Progress Toward Atomtronics Sagnac Interferometer. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28645)

Kim, H., K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple round-trip waveguide atom interferometer. Presented at *APS DAMOP 2020*, Portland, Oregon, United States, 2020-06-01 - 2020-06-01. (LA-UR-20-23957)

Kurkcuoglu, D. M. Unconventional color superfluidity in ultra-cold fermions: Quintuplet pairing, quintuple point and pentacriticality. Presented at *39th CNLS Strongly Correlated Systems Conference*, Santa Fe, New Mexico, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-23837)

Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces

Abul Azad
20180062DR

Project Description

Modern communication, sensing, and surveillance systems rely heavily on the utilization of the electromagnetic spectrum for collecting information, controlling instruments, and making decisions. Our proposed spatio-temporal modulated metasurfaces will result in a revolutionary design paradigm that will enable the effective control and manipulation of electromagnetic waves, and hence play a critical role in attaining enhanced performance of electromagnetic systems. In particular, we will apply this technology to small satellite platforms, an emerging geo-spatial capability for remote sensing and imaging which are a key component of Los Alamos National Laboratory mission space in Science of Signatures. However, they are intrinsically constrained in size, weight, and power, and are in dire need of revolutionary design paradigms to enable dramatically increased performance. This project underpins the Laboratory mission in Science supporting National Security, and advances sensing capabilities for space situational awareness in Global Security. The main anticipated outcomes of this research are reprogrammable microwave metasurface antennas for active beam steering and wavefront correction, and control over their transmission and reception characteristics through tailored modulations in space and time.

Publications

Journal Articles

Banerjee, S., N. L. Abhishikth, S. Karmakar, D. Kumar, S. Rane, S. Goel, A. K. Azad and D. R. Chowdhury. Modulating Extraordinary Terahertz Transmissions in Multilayer Plasmonic Metasurfaces. Submitted to *Journal of Optics*. (LA-UR-20-27953)

*Cardin, A. E., S. R. Silva, S. R. Vardeny, W. J. Padilla, A. Saxena, A. J. Taylor, W. J. M. Kort-Kamp, H. Chen, D. A. R. Dalvit and A. K. Azad. Surface-wave-assisted nonreciprocity in spatio-temporally modulated metasurfaces. 2020. *Nature Communications*. **11** (1): 1469. (LA-UR-19-30765 DOI: 10.1038/s41467-020-15273-1)

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Reports

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Presentation Slides

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Azad, A. K. Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces. . (LA-UR-19-20934)

Azad, A. K. LDRD-DR appraisal. . (LA-UR-20-21824)

Azad, A. K., A. E. Cardin, S. R. M. Silva and S. R. Vardeny. Dynamic metasurfaces. . (LA-UR-19-20931)

Azad, A. K. and S. R. Vardeny. LDRD-DR presentation. . (LA-UR-20-21825)

Chen, H. Few-Layer THz Metasurfaces for Effective Control of Amplitude, Phase and Polarization States. Presented at *The 4th International Symposium on Microwave/Terahertz Science and Applications & the 8th International*

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Chen, H. Narrowband Terahertz Bandpass Filters Based on Metasurfaces. Presented at *SPIE Defense + Commercial Sensing*, Orlando, Florida, United States, 2018-04-15 - 2018-04-19. (LA-UR-18-23323)

Chen, H. Hybrid Graphene Metasurfaces for High-Speed Mid-Infrared Modulation. Presented at *The 5th International Conference on Frontiers of Plasmonics (FOP5)*, Nanjing, China, 2018-04-20 - 2018-04-24. (LA-UR-18-23324)

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Chen, H. Broadband THz Linear Polarization Rotation and Linear-to-Circular Polarization Conversion Using Metasurfaces. Presented at *OSA Advanced Photonics Congress*, Zurich, Swaziland, 2018-07-02 - 2018-07-05. (LA-UR-18-25397)

Chen, H. Hybrid Graphene Metasurface for High-Speed Mid-Infrared Light Modulation and Single-Pixel Imaging. Presented at *META 2018*, Marseille, France, 2018-06-24 - 2018-06-24. (LA-UR-18-26353)

Chen, H. Achromatic Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. . (LA-UR-19-20968)

Chen, H. Metasurfaces for Manipulating Terahertz Radiation. . (LA-UR-19-25954)

Chen, H. Hybrid Graphene Metasurfaces for High-Speed Mid-Infrared Light Modulation and Single-Pixel Imaging. Presented at *ICMAT 2019*, Singapore, Singapore, 2019-06-24 - 2019-06-24. (LA-UR-19-25955)

Chen, H. Metasurfaces – Achromatic Polarization Conversion and Efficient Optical Modulation. Presented at *Seminar at Argonne National Laboratory*, Lemont, Illinois, United States, 2019-09-11 - 2019-09-11. (LA-UR-19-29185)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversions. Presented at *MTSA 2019*, Busan, Korea, South, 2019-09-30 - 2019-09-30. (LA-UR-19-29968)

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)

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Saxena, A. B. Nonreciprocity and broken symmetry in photonics: Implications for materials. Presented at *SPIE Optics and Photonics Congress*, San Diego, California, United States, 2018-08-20 - 2018-08-20. (LA-UR-18-27771)

M. Silva, S. R., W. J. de Melo Kort-Kamp, D. A. R. Dalvit, J. J. Rushton, A. K. Azad and H. Chen. Metasurface-based Static Reflectarray Antenna. . (LA-UR-19-20933)

Vardeny, S. R. and A. K. Azad. Testbeds for Active/Dynamic Metamaterial Antennas (ADMA). Presented at *DR Review*, Los Alamos, New Mexico, United States, 2020-02-25 - 2020-02-25. (LA-UR-20-21849)

Posters

Azad, A. K., S. Kramadhati, S. R. M. Silva, N. S. Sirica and H. Chen. Flat Ultrathin Metasurface Parabolic Reflector for THz Applications. . (LA-UR-19-20932)

Cardin, A. E., S. R. M. Silva, S. R. Vardeny, H. Chen and A. K. Azad. Agile Metasurfaces for Beam Manipulation. Presented at *LANL 2019 Student Symposium*, Loa Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27733)

Chen, H., A. D. Tang, S. R. M. Silva, P. L. Cantu, P. Nath and C. Corbella Bagot. Development of an Alvarez metalens in the microwave regime. . (LA-UR-19-20970)

de Melo Kort-Kamp, W. J. Topological Phase Transitions in the Photonic Spin Hall Effect. . (LA-UR-19-20927)

Saxena, A. B. Nonreciprocity and Broken Symmetry. . (LA-UR-19-20944)

Vardeny, S. R. Phase Distribution Surface Controller for Spatio-Temporal Modulated Metasurface Antennas. Presented at *DR Review*, Los Alamos, New Mexico, United States, 2019-02-05 - 2019-02-05. (LA-UR-19-20953)

Hyperspectral Xray Imaging (HXI): Nanochemical Analysis of Actinide and Explosive Materials

Mark Croce
20190002DR

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.

Publications

Journal Articles

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. Collective spin and orbital excitations in a canonical orbital system KCuF3. Submitted to *Physical Review Letters*. (LA-UR-20-27035)

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, C. M. Smith and K. E. Koehler. High-Resolution Chemical-State Mapping and Analysis for Nuclear Safeguards with Microcalorimeter SEM-EDS. Presented at *Microscopy and Microanalysis 2020*, Virtual, New Mexico, United States, 2020-08-02 - 2020-08-07. (LA-UR-20-25285)

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)

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. 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)

Posters

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)

Other

Carpenter, M. H. and M. P. Croce. HXI X1 Data as of November 2019. Dataset. (LA-UR-19-31890)

A Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) Future

Scott Twary
20190167DR

Project Description

Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/CRISPR-associated (Cas) genome engineering is rapidly advancing into all aspects of biology. This work will explore the application of novel CRISPR engineering techniques to regulate stem cell differentiation into muscle and neuron cells. Controlled interactions of these cells will then form functional neuromuscular junctions (NMJs). Effective optimized development of functional NMJs has application to traumatic injury repair, disease therapy, chemical agent testing platforms, and advanced cell biology. Varied genome engineering approaches will create multiple clonal cell lines for in depth characterization of cellular responses to targeted genetic engineering. These lines will be sequenced for genomic modifications, gene regulation responses, gene expression changes, and cellular physical response variation. The integrated analysis will provide a foundational basis for identifying aberrant cell responses to targeted genome engineering. Optimized differentiation of stem cells will provide a capability resource that will enhance biomedical applications, develop chem/bio testing platforms, and advance understanding of genetic responses.

Publications

Journal Articles

Jacobs, L. L. Soil Prokaryotic Cell Size Correlates with Ecosystem Productivity. Submitted to *Soil Biology & Biochemistry*. (LA-UR-19-31347)

Micheva-Viteva, S. N., E. A. Solomon, K. L. Davis-Anderson, S. N. Twary and R. S. Iyer. Global Transcriptome Profile of the Developmental Principles of in vitro iPSC-to-Motor Neuron Differentiation. Submitted to *BMC Neuroscience*. (LA-UR-20-28466)

Pellenz, S., M. Phelps, W. Tang, B. Hovde, R. Sinit, W. Fu, H. Li, E. Chen and R. Monnat. New human chromosomal safe harbor sites for genome engineering with CRISPR/Cas9, TAL effector and homing endonucleases. Submitted to *Human Gene Therapy*. (LA-UR-19-20028)

Strickland, J. B., K. L. Davis-Anderson, R. S. Iyer, J. F. Harris and E. A. Solomon. Applications of in vitro neuromuscular junctions for high-throughput screening and disease modeling. Submitted to *Tissue Engineering*. (LA-UR-20-27627)

Reports

Hovde, B. and J. K. Jurss. Computationally locating off-target effects of CRISPR/Cas9 in human embryonic stem cells. Unpublished report. (LA-UR-19-28097)

Presentation Slides

Davis-Anderson, K. L., S. N. Micheva-Viteva, J. F. Harris, R. S. Iyer and S. N. Twary. CRISPR-Cas9 Reprogramming of Human Stem Cells into Motor Neurons. Presented at *International Society on Stem Cell Research*, virtual, New Mexico, United States, 2020-06-23 - 2020-06-27. (LA-UR-20-24356)

Hovde, B. and J. K. Jurss. Presentation - Computationally detecting real off-target effects of CRISPR/Cas9 using NGS data. Presented at *Sequencing, Finishing, and Analysis in the Future Meeting*, Santa Fe, New Mexico, United States, 2020-12-01 - 2020-12-03. (LA-UR-20-29659)

Hraber, P. T. Cyberbiosecurity: \xe2\x80\xa8Emerging Research Field \xe2\x80\xa8or Movie-Plot Threat?. Presented at *UNM Computer Science Department Seminar*, Albuquerque, New Mexico, United States, 2019-09-25 - 2019-09-25. (LA-UR-19-29607)

Hraber, P. T. Cyberbiosecurity: \xe2\x80\xa8Emerging Research Field \xe2\x80\xa8or Movie-Plot Threat?. Presented at *UNM Computer Science Department Seminar*, Albuquerque, New Mexico, United States, 2019-09-25 - 2019-09-25. (LA-UR-19-29643)

Posters

Davis-Anderson, K. L., S. N. Micheva-Viteva, E. A. Solomon, J. C. Sanchez, S. N. Twary and R. S. Iyer. CRISPR-Cas9 Directed Reprogramming of Stem Cells into Motor Neurons for Neuromuscular Junction Organoid. Presented at *2019 CBD S&T Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-31218)

Davis-Anderson, K. L., S. N. Micheva-Viteva, J. F. Harris, R. Iyer and S. N. Twary. CRISPR-Cas9 Reprogramming of Human Stem Cells into Motor Neurons. Presented at *Cold Spring Harbor Laboratory: Genome Engineering CRISPR Frontiers*, Virtual, New Mexico, United States, 2020-08-19 - 2020-08-21. (LA-UR-20-26391)

Davis-Anderson, K. L., S. N. Micheva-Viteva, J. F. Harris, R. S. Iyer and S. N. Twary. CRISPR-Cas9 Reprogramming of Human Stem Cells into Motor Neurons. Presented at *International Society on Stem Cell Research*, virtual, New Mexico, United States, 2020-06-23 - 2020-06-27. (LA-UR-20-24355)

Hovde, B. and J. K. Jurss. CRISPR Off-Target Damage Analysis. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27822)

Hovde, B. and J. K. Jurss. Computationally detecting real off-target effects of CRISPR/Cas9 using NGS data. Presented at *Sequencing, Finishing, and Analysis in the Future Meeting*, Santa Fe, New Mexico, United States, 2020-12-01 - 2020-12-03. (LA-UR-20-29658)

Rodriguez, A. M. Motor Neuron Differentiation from Human Embryonic Stem Cells. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-26136)

Sanchez, J. C., E. A. Solomon, K. L. Davis-Anderson, S. N. Micheva-Viteva, R. S. Iyer and S. N. Twary. The conversion of human iPSCs into myocytes via CRISPR/Cas9 technology. Presented at *CSHL Genome Engineering: CRISPR Frontiers*, Cold Spring Harbor, New York, United States, 2020-08-19 - 2020-08-21. (LA-UR-20-26210)

Sanchez, J. C., K. L. Davis-Anderson, E. A. Solomon, R. S. Iyer, S. N. Micheva-Viteva and S. N. Twary. The development of a model for the human neuromuscular junction. Presented at *Cell Symposia: Engineering Organoids and Organs*, San Diego, California, United States, 2019-08-25 - 2019-08-27. (LA-UR-19-28075)

Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter

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20200035DR

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.

Publications

Journal Articles

Carrico, C., T. Capek, K. J. Gorkowski, J. T. Lam, S. Gulick, J. M. Karacaoglu, J. E. Lee, C. Dungan, A. C. Aiken, T. Onasch, A. Freedman, C. Mazzoleni and M. K. Dubey. Humidified Single Scattering Albedometer (H-CAPSPMSSA): Design, Data-Analysis, and Validation. Submitted to *Aerosol Science and Technology*. (LA-UR-21-20615)

Chylek, P., C. Folland, J. Klett, G. Lesins and M. K. Dubey. Volcanic eruptions, climate models, and climate geoengineering. Submitted to *Geophysical Research Letters*. (LA-UR-20-24163)

*Chylek, P., C. Folland, M. K. Dubey and J. D. Klett. CMIP5 Climate Models Overestimate Cooling by Volcanic Aerosols. 2020. *Geophysical Research Letters*. **47** (3): e2020GL087047. (LA-UR-19-32146 DOI: 10.1029/2020GL087047)

Josephson, A. J., D. Castano, E. Koo and R. R. Linn. Zonal-Based Emission Source Term Model for Predicting Particulate Emission Factors in Wildfire Simulations. 2020. *Fire Technology*. (LA-UR-19-27624 DOI: 10.1007/s10694-020-01024-7)

*Lee, J. E., M. K. Dubey, A. C. Aiken, P. Chylek and C. M. Carrico. Optical and Chemical Analysis of Absorption Enhancement by Mixed Carbonaceous Aerosols in the 2019 Woodbury, AZ, Fire Plume. 2020. *Journal of Geophysical Research: Atmospheres*. **125** (15): e2020JD032399. (LA-UR-20-20021 DOI: 10.1029/2020JD032399)

McClanahan, T. C., J. T. Goorley and J. D. I. Auxier. Hiroshima and Nagasaki Verification of an Unstructured Mesh based Transmutation Toolkit. Submitted to *Nuclear Technology*. (LA-UR-19-31806)

McClanahan, T. C., J. T. Goorley and J. D. I. Auxier. Comparison of Isotopic Ratios in an Urban Post-Detonation Environment. Submitted to *Journal of Radiation Effects Research and Engineering*. (LA-CP-20-20283)

*Reisner, J., E. Koo, E. Hunke and M. Dubey. Reply to Comment by Robock et al. on “Climate Impact of a Regional Nuclear Weapon Exchange: An Improved Assessment Based on Detailed Source Calculations”. 2019. *Journal of Geophysical Research: Atmospheres*. **124** (23): 12959-12962. (LA-UR-19-26224 DOI: 10.1029/2019JD031281)

Conference Papers

McClanahan, T. C. Study of the Production of Radionuclides in Polluted Air from an Urban Nuclear Detonation. Presented at *RPSD 2020*. (Seattle, Washington, United States, 2020-09-13 - 2020-09-17). (LA-UR-20-22003)

Reports

Dubey, M. K., J. J. Benedict, D. O'Malley, B. T. Nadiga, P. A. Johnson, H. S. Viswanathan, P. Chylek and S. Carns. AI for Extreme Volcanic Climate Forcing and Feedback Forecasting in the 21st century. Unpublished report. (LA-UR-21-21384)

Dunning, D. J. Parallelization and Performance Portability in Hydrodynamics Codes. Unpublished report. (LA-UR-20-27394)

Elliott, S. M., C. S. Plesko, T. M. Holland, M. K. Dubey, J. M. Reisner, J. H. Cooley, A. C. Aiken, G. D'Angelo, W. P. Even, C. L. Fryer, G. R. Gisler, K. J. Gorkowski, R. C. Huber, A. J. Josephson, C. M. Mauney, T. C. McClanahan, R. A. Messerly, E. Rougier and E. M. Whitney. Chemistry of Pulses to the Earth Surface Environment: Overview for Next Generation Simulation. Unpublished report. (LA-UR-20-26027)

McClanahan, T. C. Study of the Production of Isotopes in an Urban Nuclear Post-Detonation Environment. Unpublished report. (LA-UR-20-21439)

Presentation Slides

Aiken, A. C., R. C. Huber, A. M. Schmalzer, M. A. Boggs, J. E. Lee, K. J. Gorkowski and M. K. Dubey. Submicron Soot Microphysical and Chemical Signatures from Detonations of High Explosive Composites. Presented at *38th Annual American Association for Aerosol Research Conference - Virtual Meeting*, Los Alamos, New Mexico, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-27497)

Brown, A. L., H. Mendoza, E. Koo and J. M. Reisner. A High Flux Forest Fire Scenario for Assessing Relative Model Accuracy for CFD Tools. Presented at *Western States Section Combustion Institute (WSSCI)*, Albuquerque, New Mexico, United States, 2019-10-14 - 2019-10-15. (LA-UR-19-30060)

Dubey, M. K. Field Observations of Climate Forcing by Fires, Forests, Fossil Energy & Food Production. Presented at *Texas A&M University Atmospheric Science Seminar*, College Station, Texas, United States, 2020-01-29 - 2020-01-29. (LA-UR-20-20735)

Dubey, M. K., A. C. Aiken, K. J. Gorkowski, J. E. Lee, T. Capek and C. Carrico. TRacking Aerosol Convection interactions ExpeRiment (TRACER): Carbon Aerosol Thrust (CAT). Presented at *ARM TRACER WORKSHOP (Virtual)*, Los Alamos, New Mexico, United States, 2020-04-20 - 2020-04-21. (LA-UR-20-22994)

Dubey, M. K., J. M. Reisner, E. Koo, S. Guimond, A. C. Aiken, G. D'Angelo, D. Peterson and M. Fromm. Transport, Composition and Lifetime of Extreme Wildfire Smoke to Assess their Impacts. Presented at *AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32202)

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)

Dubey, M. K. and J. M. Reisner. Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter. Presented at *LDRD-DR 1st year progress review*, Los Alamos, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20046)

Josephson, A. J., E. Koo, D. K. Thompson and J. M. Reisner. Aerosol Formation and Ejection via Pyrocumulonimbus Clouds in the British Columbia Fires of Late Summer 2017. Presented at *AAAR 38th Annual Conference*, Los Alamos, New Mexico, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-28540)

Josephson, A. J. and R. R. Linn. Modeling Soot Emissions in Coarse Grid Simulations. Presented at *2019 Fall Technical Meeting of the Western States Section of the Combustions Institute*, Albuquerque, New Mexico, United States, 2019-10-14 - 2019-10-15. (LA-UR-19-30398)

Koo, E. LDRD-DR Project: Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter. Presented at *Invited Talk to Mechanical Engineering Dept, University of New Mexico.*, Albuquerque, New Mexico, United States, 2021-01-29 - 2021-01-29. (LA-UR-21-20956)

Koo, E. CY2020 Institutional Computing Annual Progress Report: Multi-scale turbulent atmospheric interactions (w19_atmo_turbulence, renewed as w21_atmoturb). . (LA-UR-21-21906)

McClanahan, T. C. Study of the Production of Isotopes in an Urban Nuclear Post- Detonation Environment. . (LA-UR-20-22421)

McClanahan, T. C., J. M. Reisner, E. Koo and M. K. Dubey. Path Forward: Hiroshima Nuclear Activation, Exposure, Black Rain Fallout Simulations and Chemical Analysis. Presented at *LDRD DR Mid year Appraisal*, Los Alamos, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20076)

Perez, D. M. Cloud Microphysics Considerations for Simulating Pyrocumulonimbus Clouds in HIGRAD. . (LA-UR-20-27338)

Reisner, J. M. Towards Modeling Complex Fallout: Model Description and Preliminary Results. Presented at *JOWOG 43*, Los Alamos, New Mexico, United States, 2020-01-06 - 2020-01-06. (LA-CP-20-20000)

Reisner, J. M. Nuclear Winter Update: Post Reisner et al. (2018) JGR paper. . (LA-UR-20-23077)

Posters

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)

Aiken, A. C., R. C. Huber, A. M. Schmalzer, M. A. Boggs, J. E. Lee, K. J. Gorkowski and M. K. Dubey. High Temperature and Pressure Regime Soot Microphysical and Chemical Analysis for Real-Time Atmospheric Detection of High Explosives. Presented at *AGU Fall Meeting*, los alamos, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29713)

Dubey, M. K., P. Chylek, G. D'Angelo, S. R. Guimond and J. M. Reisner. Evaluating Aerosol Solar Reflection Climate Models by Post Stratospheric Mass Injection Response Observations. Presented at *AGU Fall Meeting*, Washington,

District Of Columbia, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29624)

Lee, J. E., M. K. Dubey, A. C. Aiken, K. J. Gorkowski and C. Carrico. Black carbon aerosol mixing state in fresh and aged wildfire smoke: Harmonizing Instruments, Laboratory and Field Studies. Presented at *AGU 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-18. (LA-UR-20-29833)

Other

Lee, J. E., M. K. Dubey and A. C. Aiken. Datafiles for: Optical and chemical analysis of absorption enhancement by mixed carbonaceous aerosols in the 2019 Woodbury, AZ fire plume. Dataset. (LA-UR-20-20454)

Capturing the Origin and Evolution of Persistence Using Real-time, In vivo, Single Cell Transcriptomics

Murray Wolinsky
20200222DR

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.

Publications

Journal Articles

Kalb, D. M., H. Vo, S. H. Adikari, E. Hong-Geller, B. munsky and J. H. Werner. Visualization and Modeling of Inhibition of IL-1\xce\xb2 and TNF\xce\xb1 mRNA Transcription at the Single-Cell Level. Submitted to *Scientific Reports*. (LA-UR-20-28135)

Conference Papers

Strauss, C. E. and J. Morton. Protein Structural Alignments From Sequence. Presented at *NeuroIPS: Thirty-fourth Conference on Neural Information Processing Systems*. (Virtual, New Mexico, United States, 2020-12-06 - 2020-12-12). (LA-UR-20-28603)

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)

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)

The Remote Elemental, Molecular, and Isotopic Camera (REMICam)

Samuel Clegg
20200770DR

Project Description

The Remote Elemental, Molecular, and Isotopic Camera (REMICam) instrument is a suite of analytical techniques capable of remote chemical, molecular and isotopic analysis in the field. REMICam integrates Laser-Induced Breakdown Spectroscopy (LIBS), Time Resolved Raman Spectroscopy (Raman), Time-Resolved Luminescence Spectroscopy (TRLS), and Visible and Near Infrared Spectroscopy (VisNIR) into a single instrument. REMICam is based on the ChemCam instrument currently operating on the National Aeronautics Space Administration (NASA) Mars Curiosity rover and the SuperCam instrument scheduled to launch on July 30, 2021 on the NASA Perseverance rover. While ChemCam and SuperCam are designed to operate under the reduced martian surface temperature and pressure, REMICam will be the first instrument of its kind to operate under Earth ambient surface temperatures and pressures. This project will discover a new ensemble of signatures and perform advanced quantitative analysis on them. The REMICam instrument will result in revolutionary measurement techniques for many security missions. Finally, forward deployment will be realized by the field demonstrations where REMICam will analyze various chemical, biological, radiological, nuclear, and explosive (CBRNE) samples in the field.

The Fundamental Physical Interpretation and Exploitation of Stable Isotope Fractionation

Samuel Clegg
20180066DR

Project Description

This project will theoretically and experimentally investigate the mechanisms responsible for the fractionation of stable isotopes. Stable isotopes are long-lived, non-radioactive atoms. Stable isotopes are exceedingly sensitive indicators of the source of a material and are widely used within the atmospheric chemistry, geochemical, planetary, environmental,forensic, and climate change communities. However, interpretation of stable isotope ratios is limited to empirical analysis without much detailed theoretical understanding. The proposed work will provide the fundamental tools and models necessary to relate stable isotopic signatures to specific processing steps used in their production.

Technical Outcomes

The highest-level experimental and theoretical conclusion from this project is that isotopologue analysis produces far more diagnostic information than the current state-of-the-art stable isotope analysis. Isotopologues are molecules that contain different isotopes. Isotopologue analysis requires the development of new analytical methods, such as our use of an Fourier Transform infrared spectroscopy (FTIR), as the current state-of-the-art isotope ratio mass spectrometer does not distinguish molecules with different isotopes.

Publications

Journal Articles

Babikov, D., E. Grushnikova, I. Gayday and A. Teplukhin. Four isotope-labeled recombination pathways of ozone formation. Submitted to *Journal of Chemical Physics*. (LA-UR-21-20550)

Carlson, R. K., S. M. Clegg, P. Yang and E. R. Batista. Mechanistic Study of Copper Dissolution in Nitric Acid. Submitted to *Inorganic Chemistry*. (LA-UR-20-20214)

*Currier, R. P., T. B. Peery, M. F. Herman, R. F. Williams, R. Michalczyk, T. E. Larson, D. M. Labotka, J. E. Fessenden and S. M. Clegg. Azeotropic isotopologues. 2019. *Fluid Phase Equilibria*. **493**: 188-195. (LA-UR-18-30223 DOI: 10.1016/j.fluid.2019.04.006)

*Dorhout, J. M., A. S. Anderson, E. Batista, R. K. Carlson, R. P. Currier, R. K. Martinez, S. M. Clegg, M. P. Wilkerson and K. Nowak-Lovato. NOx speciation from copper dissolution in nitric acid/water solutions using FTIR spectroscopy. 2020. *Journal of Molecular Spectroscopy*. **372**: 111334. (LA-UR-20-22646 DOI: 10.1016/j.jms.2020.111334)

Dorhout, J. M., K. L. Nowak-Lovato, A. S. Anderson, E. R. Batista, R. K. Carlson, Z. Li, R. K. Martinez, M. P. Wilkerson, S. M. Clegg and R. P. Currier. Characterization of Nitrogen-Containing Species Produced from Nitric Acid/Water Systems. Submitted to *Journal of Physical Chemistry A*. (LA-UR-19-24140)

Dorhout, J. M., K. L. Nowak-Lovato, A. S. Anderson, R. K. Martinez, Z. Li, M. P. Wilkerson and S. M. Clegg. Production of Nitrogen-Containing Species in Nitric Acid/Water Systems. Submitted to *Journal of Physical Chemistry A*. (LA-UR-19-20615)

*Dorhout, J. M., K. Nowak-Lovato, R. K. Carlson, R. P. Currier, A. S. Anderson, E. R. Batista, Z. Li, R. K. Martinez, M. P. Wilkerson and S. M. Clegg. Characterization of nitrogen-containing species produced from nitric acid/water systems. 2020. *Journal of Molecular Spectroscopy*. **371**: 111307. (LA-UR-20-20673 DOI: 10.1016/j.jms.2020.111307)

*Gayday, I., A. Teplukhin, B. K. Kendrick and D. Babikov. Theoretical Treatment of the Coriolis Effect Using Hyperspherical Coordinates, with Application to the Ro-Vibrational Spectrum of Ozone. 2020. *The Journal of Physical Chemistry A*. **124** (14): 2808-2819. (LA-UR-19-31077 DOI: 10.1021/acs.jpca.0c00893)

*Gayday, I., A. Teplukhin, B. K. Kendrick and D. Babikov. The role of rotation–vibration coupling in symmetric and asymmetric isotopomers of ozone. 2020. *The Journal of Chemical Physics*. **152** (14): 144104. (LA-UR-19-32237 DOI: 10.1063/1.5141365)

Huang, J., B. K. Kendrick and D. H. Zhang. Mechanistic Insights into Geometric Phase Effects in the Ultracold O + OH

Reaction. Submitted to *Physical Review Letters*. (LA-UR-20-28130)

*Larson, T. E., G. B. Perkins, R. F. Williams, J. E. Fessenden, S. M. Clegg and R. P. Currier. Partitioning of oxygen isotopes during the aqueous solvation of nitric acid. 2020. *Fluid Phase Equilibria*. **506**: 112364. (LA-UR-19-25191 DOI: 10.1016/j.fluid.2019.112364)

Li, Z., K. L. Nowak-Lovato, A. S. Anderson, S. M. Clegg, R. K. Martinez, J. M. Dorhout and R. K. Carlson. Sequential cryogenic separation of NOx species (NO + NO2) for online nitrogen isotopic analysis using EA-IRMS. Submitted to *Rapid Communications in Mass Spectrometry*. (LA-UR-19-20860)

M. Mallory, E. J., T. B. Peery and M. F. Francis. Statistical representations and unbiased metrics for stable isotope fractionation. Submitted to *Chemical Geology*. (LA-UR-20-20132)

Reyes-Newell, A. L., R. K. Martinez, K. L. Nowak-Lovato and S. M. Clegg. Development of a widely tunable continuous wave (CW) external cavity quantum cascade laser (EC-QCL) operating at 6.24 \xc2\xb5m. Submitted to *Optics Letters*. (LA-UR-20-27772)

*Teplukhin, A. and B. K. Kendrick. Three-dimensional potential energy surfaces of ArNO (X\xcc\x83\xe2\x80\x892\xce\xa0). 2020. *Journal of Chemical Physics*. **152** (11): 114302. (LA-UR-20-20133 DOI: 10.1063/1.5145011)

Conference Papers

Peery, T. B., R. P. Currier, E. J. M. Mallory and S. M. Clegg. Statistical Reference States in Stable Isotope Fractionation and Chemistry. Presented at *LDRD 20180066DR third-year review*. (Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15). (LA-UR-20-20149)

Books/Chapters

Clegg, S. M., K. L. Nowak-Lovato, R. P. Currier, J. E. Fessenden and R. K. Martinez. Surface Monitoring, Verification and Accounting (MVA) for Geologic Sequestration Storage. (LA-UR-18-26244)

Clegg, S. M., K. L. Nowak-Lovato, R. P. Currier, J. E. Fessenden and R. K. Martinez. Surface Monitoring, Verification and Accounting (MVA) for Geologic Sequestration Storage. (LA-UR-19-27356)

Presentation Slides

Carlson, R. K. Copper Dissolution in Nitric Acid: Unraveling a Century of Hypotheses. Presented at *ACS National Meeting*, San Diego, California, United States, 2019-08-26 - 2019-08-26. (LA-UR-19-28350)

Carlson, R. K. and E. R. Batista. Cu + HNO3 Dissolution: Mechanism and Fractionation. Presented at *DR Review*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20870)

Clegg, S. M. Venus Elemental and Mineralogical Camera (VEMCam). . (LA-UR-18-26082)

Currier, R. P., T. B. Peery, M. F. Herman, R. F. Williams, R. Michalczyk, T. E. Larson, G. B. Perkins, J. E. Fessenden, R. K. Martinez, A. L. Reyes-Newell, D. M. Labotka and S. M. Clegg. Isotopologues at an Azeotrope. Presented at *Invited Chemistry Department seminar (Tulane University)*, New Orleans, Louisiana, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30264)

Currier, R. P., T. B. Peery, M. Herman, D. M. Labotka, J. E. Fessenden, R. K. Martinez, A. L. Reyes-Newell and S. M. Clegg. Phase Equilibrium Physically or Chemically Driven Fractionation?. Presented at *Presentation for LDRD-DR Mid-Term Review Meeting*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20802)

Dorhout, J. M., K. L. Nowak-Lovato, R. K. Carlson, E. R. Batista, Z. Li, M. P. Wilkerson and S. M. Clegg. Stable-Isotope Fractionation of Nitrogen by Metals in Nitric Acid. Presented at *ACS Southwest Regional Meeting*, El Paso, Texas, United States, 2019-11-12 - 2019-11-16. (LA-UR-19-31174)

Kendrick, B. K. APH3D: A Parallel Code Suite for Computing Quantum Dynamics of A + BC Reactions and Triatomic Spectra. Presented at *2019 MolSSI Workshop on Rovibrational Molecular Spectroscopy*, Blacksburg, Virginia, United States, 2019-11-14 - 2019-11-15. (LA-UR-19-31395)

Kendrick, B. K. and A. Teplukhin. Quantum Mechanical Theory of Stable Isotope Fractionation. Presented at *DR Appraisal meeting for Fundamental Physics and Interpretation of Stable Isotope Fractionation*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20572)

Kendrick, B. K. and A. Teplukhin. Quantum Mechanical Treatment of Stable Isotope Fractionation. . (LA-UR-20-20202)

Kendrick, B. K. and A. Teplukhin. Quantum Reactive Scattering Calculations of Isotope Fractionation. . (LA-UR-21-21953)

Nowak-Lovato, K. L., J. M. Dorhout, Z. Li, R. K. Martinez and A. S. Anderson. NOx Fractionation - Experimental. . (LA-UR-19-20749)

Nowak-Lovato, K. L., R. K. Carlson, J. M. Dorhout, Z. Li, R. K. Martinez and A. S. Anderson. NOx summary. . (LA-UR-20-20477)

Teplukhin, A. and B. K. Kendrick. Ultracold scattering of Ar-NO in three dimensions. Presented at *The 51st Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Portland, Oregon, United States, 2020-06-01 - 2020-06-05. (LA-UR-20-23928)

Teplukhin, A. and B. K. Kendrick. Isotope effects in ultracold3D non-adiabatic scattering of Ar–NO. Presented at *APS March*

Meeting 2021 (virtual), College Park, Maryland, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22470)

Posters

Beveridge, A. C., K. L. Nowak-Lovato, S. M. Clegg, R. K. Martinez, A. L. Reyes-Newell, A. S. Anderson, E. R. Batista, R. K. Carlson, B. K. Kendrick and A. Teplukhin. NOx and SOx Photochemistry Experiments. Presented at *LDRD Review Meeting*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20789)

Carlson, R. K., S. M. Clegg, P. Yang and E. R. Batista. Nitrogen Isotope Fractionation During the Dissolution of Copper by Nitric Acid. Presented at *LDRD Project Review*, Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20268)

Daniel, J., K. Rodriguez, T. Lewis, S. Kelly, A. Teplukhin, B. K. Kendrick, C. Bardeen, S. W. Tsai and B. Hemmerling. Progress towards laser cooling of AlCl. Presented at *DAMOP 2020 (virtual)*, Portland, Oregon, United States, 2020-06-01 - 2020-06-01. (LA-UR-20-23930)

Dorhout, J. M., A. S. Anderson, K. L. Nowak-Lovato, R. K. Martinez, G. B. Perkins, Z. Li, M. P. Wilkerson and S. M. Clegg. Stable-Isotope Fractionation of Nitrogen Species by Copper in Nitric Acid/Water Systems. . (LA-UR-20-20391)

Dorhout, J. M., A. S. Anderson, K. L. Nowak-Lovato, R. K. Martinez, Z. Li, M. P. Wilkerson and S. M. Clegg. Production of Nitrogen Species in Nitric Acid/Water Systems. . (LA-UR-19-20603)

Dorhout, J. M., A. S. Anderson, K. L. Nowak-Lovato, R. K. Martinez, Z. Li, M. P. Wilkerson and S. M. Clegg. Stable-Isotope Fractionation of Nitrogen Species by Copper or Uranium in Nitric Acid/Water Systems. . (LA-UR-19-20606)

Dorhout, J. M., Z. Li, S. M. Clegg, K. L. Nowak-Lovato, A. S. Anderson, M. P. Wilkerson and R. K. Martinez. Stable-Isotope Fractionation of Nitrogen by Uranium in Nitric Acid. Presented at *Pu Futures*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28511)

Kendrick, B. K. and A. Teplukhin. Quantum Mechanical Description of Isotope Effects in SO2. . (LA-UR-20-20203)

Labotka, D. M., G. B. Perkins, R. P. Currier and S. M. Clegg. Oxygen-17 Fractionation Dynamics. . (LA-UR-19-20619)

Li, Z., K. L. Nowak-Lovato, A. S. Anderson, J. M. Dorhout, R. K. Carlson, R. K. Martinez and S. M. Clegg. Cryogenic separation of NOx species (NO + NO2) for on-line nitrogen isotopic analysis using EA-IRMS. . (LA-UR-19-20835)

Li, Z., K. L. Nowak-Lovato, A. S. Anderson, J. M. Dorhout, R. P. Currier, S. M. Clegg, R. K. Martinez and R. K. Carlson. Sequential cryogenic separation and purification of NOx species (NO + NO2) for on-line nitrogen isotopic analysis using EA-IRMS. . (LA-UR-20-20022)

Peery, T. B., E. J. M. Mallory, R. P. Currier, M. F. Herman and S. M. Clegg. On Statistics & Standard Reference States in the Fractionation of Stable Isotopes. Presented at *LDRD-DR 20180066DR mid-term review at LANL*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20703)

Peery, T. B., E. J. M. Mallory, R. P. Currier and S. M. Clegg. Statistical Reference States in Stable Isotope Fractionation and Chemistry. Presented at *LDRD 20180066DR Third-Year Internal Review*, Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20153)

Teplukhin, A. and B. K. Kendrick. Quantum mechanical description of isotope effects in ArNO and NO2. Presented at *LDRD project review*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20518)

Teplukhin, A. and B. K. Kendrick. Quantum mechanical description of isotope effects in ArNO and NO2. Presented at *LDRD project review*, Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20204)

Teplukhin, A. and B. K. Kendrick. Bound states calculation for ArNO on a three-dimensional potential energy surface. Presented at *The 67th Pacific Conference on Spectroscopy and Dynamics*, San Diego, California, United States, 2020-01-30 - 2020-02-02. (LA-UR-20-20507)

Dose and Signature Assessment for Triage Applications

Jennifer Harris
20200040DR

Project Description

After the fall of the Soviet Union, the United States largely abandoned research funding of health effects of non-medical radiation. Since then, new nuclear programs have arisen in hostile countries, an earthquake and tsunami caused a disastrous radiation release from reactors at the Fukushima Dai-ichi nuclear power plant, and a shocking number of radioactive medical treatment devices are missing. Given that much of our data to guide radiation health response is outdated, there is a need to update our models, and discover new biomarkers that can help guide medical response. Human 3-Dimensional laboratory-cultured organs re-create organ functions and are a potential bridge between animal studies and humans. They can be utilized in situations where animal research would be inhumane, and human research would be unethical. We will utilize organ cultures to give us modern insights into human radiation biology. This project will complete a publishable pilot study to validate that exposure of 3D laboratory organs to low dose ionizing radiation recapitulates human responses identified in literature. Showing that 3D organ cultures can recapitulate known responses to ionizing radiation will establish the utility of these model systems for assessment of accidental environmental dispersals, medical imaging and treatment, and potential hostile threats.

Technical Outcomes

A major technical outcome of this project was the verification of 3-dimensional laboratory organ cultures as a viable model for human response to radiation. The team exposed laboratory-cultured organ tissues to radiation doses similar to medical doses utilized in whole-body radiation therapy. The transcriptome, or regulation of genes from the treated organ samples was compared to known results from literature and known patient data. The radiation activated the same pathways in the organs as in patients.

Publications

Presentation Slides

Harris, J. F. Expanding the Potential of 3D Organ Cultures. . (LA-UR-20-26587)

Basic Science Influencing Emplacement Signatures of Underground Nuclear Explosions

Thomas Rahn
20200092DR

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.

Technical Outcomes

This project successfully used the Nuclide Inventory Model to make preliminary assessments of the effects of neutron flux on non-traditional aspects of the Trinity test and developed analytical methods and performed analysis on samples from Trinity Site demonstrating that anomalous isotopic signatures are observed. The work completed to date has allowed the team to demonstrate the viability of pursuing this avenue of research at a higher level.

Imaging Neural Dynamics With Ultra-Low Field Magnetic Resonance Imaging (MRI)

Per Magnelind
20180058ER

Project Description

This project will provide a new neuroimaging capability that will aid in different aspects of increasing the knowledge about the most complex system we know – the human brain. An increased fundamental understanding of the brain would have important implications in the vast field of neuroscience (e.g. within National Institutes of Health – NIH), and could have importance for national security by enhancing human performance through methods such as transcranial electrical stimulation and magnetic stimulation, which are of interest to numerous Department of Defense (DoD) sponsors, such as the Defense Advanced Research Projects Agency (DARPA).

Publications

Presentation Slides

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-17-29752)

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-19-31476)

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Ultra-low field MRI and Current Density Imaging. Presented at *SBMT2018*, Los Angeles, California, United States, 2018-04-13 - 2018-04-13. (LA-UR-18-23160)

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Current-density imaging and magnetic resonance-based electrical impedance tomography at ultra-low fields. Presented at *Biomag2018*, Philadelphia, Pennsylvania, United States, 2018-08-26 - 2018-08-30. (LA-UR-18-28117)

Posters

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Current-density imaging and magnetic resonance-based electrical impedance tomography at ultra-low fields. Presented at *Biomag2018*, Philadelphia, Pennsylvania, United States, 2018-08-26 - 2018-08-30. (LA-UR-18-28116)

Proton Radiography for Advanced Cancer Therapy

Michelle Espy
20180238ER

Project Description

More than two dozen proton therapy centers now operate in the US, taking advantage of the centimeter precision while minimizing the radiation absorbed in nearby healthy tissue. Even more precise proton treatments could target tumors on the order of a millimeter in size, or to tumors close to sensitive tissues, if relativistic proton beams(~1GeV) were used. The future of proton beam therapy will be at high energy, with direct, positive impact in treating the most difficult cancers, including some that may have otherwise been deemed untreatable, and those in the most radiation-sensitive, pediatric patients. Fully exploiting the precision of the higher-energy protons will require imaging both the patient and the dose deposition in real-time, on location, to ensure radiation accurately targets the tumor during each treatment. Fortunately, the same relativistic protons used for treatment can also be used to image tumors in a patient, as well as track treatment delivery. We propose to use the LANSCE Proton Radiography Facility (pRad) to demonstrate imaging of small tagged tumors in mice with sufficient resolution and low enough dose to guide precise relativistic proton beam therapy. This work could profoundly influence the future development of proton therapy worldwide.

Publications

Journal Articles

Freeman, M. S., E. F. Aulwes, M. A. Espy, J. F. Hunter, P. E. Magnelind, F. E. Merrill, F. R. Trouw and D. Tupa. Direct Proton Detection for Therapy Guidance and Treatment Planning. Submitted to *Medical Physics*. (LA-UR-18-30411)

Freeman, M. S., F. E. Merrill, J. C. Allison, E. F. Aulwes, M. G. Davis, P. E. Magnelind, F. G. Mariam, L. I. Martinez, J. J. Medina, W. Z. Meijer, L. P. Neukirch, T. Schurman, R. B. Sidebottom, Z. Tang, F. R. Trouw, D. Tupa, J. L. Tybo and M. A. Espy. Dark Field Proton Radiography. Submitted to *Applied Physics Letters*. (LA-UR-20-23116)

Sidebottom, R. B., J. C. Allison, E. F. Aulwes, B. A. Broder, M. S. Freeman, P. E. Magnelind, F. G. Mariam, F. E. Merrill, L. P. Neukirch, T. Schurman, Z. Tang, D. Tupa, J. L. Tybo, C. H. Wilde and M. A. Espy. Gold leaf phantom development for the assessment of proton radiographic sensitivity limits simulating gold nanoparticle tagged tumors. Submitted to *Journal of Medical Imaging*. (LA-UR-20-28481)

Conference Papers

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. G. Mariam, F. E. Merrill, D. Tupa and C. H. Wilde. Proton Radiography for Relativistic Proton Beam Therapy. Presented at *SPIE Medical Imaging*. (Houston, Texas, United States, 2018-02-12 - 2018-02-16). (LA-UR-18-20428)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, F. E. Merrill, P. E. Magnelind, D. Tupa and M. A. Espy. Gold nanoparticles for tumor detection with proton radiography: optimizing sensitivity and determining detection limits. Presented at *SPIE Photonics West*. (Virtual, New Mexico, United States, 2021-03-06 - 2021-03-06). (LA-UR-21-20944)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill, D. Tupa and M. A. Espy. Assessment of proton radiographic sensitivity limits for gold nanoparticle tagged tumors using gold leaf phantoms. Presented at *SPIE Medical Imaging*. (Houston, Texas, United States, 2020-02-16 - 2020-02-16). (LA-UR-20-20414)

Reports

Sidebottom, R. B. Gold-leaf phantoms of Au-tagged tumors to assess proton radiography for image guided proton therapy. Unpublished report. (LA-UR-19-23315)

Presentation Slides

Broder, B. A. Simulating Contrast in LANSCE's pRad System via TOPAS. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-26128)

Broder, B. A. Summary: LANL 2020 Internship. . (LA-UR-20-27155)

Espy, M. A. How to look at a brain. Presented at *NogginFest*, portland, Oregon, United States, 2018-10-19 - 2018-10-20. (LA-UR-18-29895)

Freeman, M. S. Magnetic focused proton radiography and its implications for proton beam guidance, anatomical alignment and adaptive therapy. Presented at *Annual*

Rocky Mountain Chapter Meeting of the American Association of Physicists in Medicine, Colorado Springs, Colorado, United States, 2018-06-09 - 2018-06-09. (LA-UR-18-24975)

Freeman, M. S. Instantaneous Full Field Proton Radiography For Image Guidance. Presented at *American Association of Physicists in Medicine*, Nashville, Tennessee, United States, 2018-07-29 - 2018-08-02. (LA-UR-18-25530)

Freeman, M. S. Proton Radiography for Treatment Planning and Guidance. Presented at *UNM Medical Physics Symposium*, Albuquerque, New Mexico, United States, 2018-11-16 - 2018-11-16. (LA-UR-19-20477)

Freeman, M. S. Flash Proton Radiography for the Clinic: Real-Time Adaptive Therapy and a Proton-Based Estimate of Water-Equivalent Thickness. . (LA-UR-19-23520)

Freeman, M. S. Proton Radiography for Dense Dynamic Systems: a Capabilities Overview. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-31068)

Freeman, M. S. Hyperpolarized 129Xe MRI: Visualizing Lung Anatomy and Function. . (LA-UR-19-31585)

Freeman, M. S. Spin Physics. . (LA-UR-20-26492)

Freeman, M. S. Hyperpolarized 129Xe MRI Visualizing Lung Anatomy and Function. . (LA-UR-20-29731)

Freeman, M. S., E. F. Aulwes, L. Dong, T. Li, P. E. Magnelind, F. E. Merrill, L. P. Neukirch, R. Selwyn, R. Serda, R. B. Sidebottom, Z. Tang, K. Teo, D. Tupa, C. H. Wilde and M. A. Espy. Scaling the Ultra-Fast LANL System to Medical Energies. Presented at *58th Annual Meeting of the Particle Therapy Co-Operative Group*, Manchester, United Kingdom, 2019-06-10 - 2019-06-10. (LA-UR-19-25360)

Freeman, M. S., E. F. Aulwes, L. Dong, T. Li, P. E. Magnelind, F. E. Merrill, R. Selwyn, R. Serda, R. B. Sidebottom, K. Teo, D. Tupa and M. A. Espy. Residual-Energy Lens Focused Proton Radiography at Clinical Energies. Presented at *Annual Meeting of the American Association of Physicists in Medicine*, San Antonio, Texas, United States, 2019-07-14 - 2019-07-14. (LA-UR-19-26544)

Freeman, M. S., J. C. Allison, M. A. Espy, J. J. I. Goett, J. D. Lopez, P. E. Magnelind, F. G. Mariam, J. J. Medina, F. E. Merrill, C. Morris, L. P. Neukirch, A. Saunders, A. M. Tainter, Z. Tang, F. R. Trouw, D. Tupa, J. L. Tybo and C. H. Wilde. Instantaneous Full Field Proton Radiography for Image Guidance. Presented at *Annual Meeting of the American Association of Physicists in Medicine*, Nashville, Tennessee, United States, 2018-07-22 - 2018-07-22. (LA-UR-18-26984)

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. E. Merrill and D. Tupa. Proton Radiography and Therapy. . (LA-UR-18-22459)

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-19-31476)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill, D. Tupa and M. A. Espy. Gold nanoparticles for tumor detection with proton radiography: optimizing sensitivity and determining detection limits. Presented at *SPIE Photonics West BiOS*, Virual, New Mexico, United States, 2021-03-06 - 2021-03-11. (LA-UR-21-21067)

Posters

Aulwes, E. F., M. S. Freeman, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. A. Espy. Developing a Treatment Planning Method for High-Energy Proton Therapy. . (LA-UR-19-27480)

Broder, B. A. and M. S. Freeman. TOPAS Model for Simulating Proton Radiography. Presented at *Research Computing Expo and Symposium*, chicago, Illinois, United States, 2019-11-05 - 2019-11-05. (LA-UR-19-30818)

Freeman, M. S., E. F. Aulwes, P. E. Magnelind, F. E. Merrill, L. P. Neukirch, R. B. Sidebottom, Z. Tang, D. Tupa and C. H. Wilde. Water Equivalent Thickness from Instantaneous Proton Radiographic Transmission Measurements. Presented at *International Meeting of the Particle Therapy Co-Operative Group*, Manchester, United Kingdom, 2019-06-10 - 2019-06-10. (LA-UR-19-25169)

Freeman, M. S., M. A. Espy, J. J. I. Goett, P. E. Magnelind, F. G. Mariam, F. E. Merrill, R. B. Sidebottom, F. R. Trouw, D. Tupa and C. H. Wilde. Lens-Refocused Proton Radiography for Proton Beam Guidance. Presented at *Annual Meeting 57 of the Proton Therapy Co-Operative Group*, Cincinnati, Ohio, United States, 2018-05-21 - 2018-05-26. (LA-UR-18-23884)

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. G. Mariam, F. E. Merrill, D. Tupa and C. H. Wilde. Proton Radiography for Relativistic Proton Beam Therapy. Presented at *SPIE Medical Imaging 2018*, Houston, Texas, United States, 2018-02-12 - 2018-02-16. (LA-UR-18-20846)

Sidebottom, R. B., D. Tupa, E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill and M. A. Espy. Gold-leaf phantoms of AuNP-tagged tumors to assess proton radiography for image-guided proton therapy. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27565)

Sidebottom, R. B., D. Tupa, E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill and M. A. Espy. Assessment of proton radiographic sensitivity limits for gold nanoparticle tagged tumors using gold leaf phantoms. Presented at *SPIE Medical Imaging*, Houston, Texas, United States, 2020-02-16 - 2020-02-16. (LA-UR-20-20412)

OrganiCam: A High-Sensitivity Radiation-Hardened Imaging Organic Detector For Space and Programmatic Applications

Roger Wiens
20180244ER

Project Description

This is a dual-purpose project with applications for outer solar system and for high-radiation areas on Earth such as nuclear reactor cores or an accident area such as Fukushima. We plan to build a time-resolved fluorescence camera and spectrometer (OrganiCam) that will be able to observe and distinguish organic and mineral (e.g., heavy-element) fluorescence. In tune with the NASA applications, we will study and develop plans for an instrument that can survive and operate in a highly radioactive environment. Robots like the "Little Sunfish" now exploring the insides of the Fukushima reactor show that instruments of this type can be highly beneficial in surveying damage in a nuclear contamination zone. Careful use of electronic and optical components are required for such an environment and so our project will focus significant effort for this capability.

Publications

Journal Articles

Gasda, P. J., R. C. Wiens, A. L. Reyes-Newell, K. Ganguly, R. T. Newell, C. G. Peterson, B. F. Sandoval, L. A. Ott, S. H. Adikari, S. J. Voit, S. M. Clegg, A. Misra, T. Acosta-Maeda, H. M. Quinn, S. Sharma, M. E. Dale, S. P. Love and S. Maurice. OrganiCam: a lightweight time-resolved laser-induced luminescence imager and Raman spectrometer for planetary organic material characterization. Submitted to *Applied Optics*. (LA-UR-21-20845)

Presentation Slides

Ganguly, K., P. J. Gasda, C. D. Gleasner, C. Mensah, S. H. Adikari, H. M. Quinn, A. C. Watkins, S. P. Love, A. Misra, T. Acosta-Mayda, S. K. Sarma and R. C. Wiens. Survival, Genetic Modification, and Time-Resolved Laser-Induced Fluorescence Analysis of Bacteria Exposed to High-Dose Radiation Simulating Europa's Surface. Presented at *Europa Workshop*, Houston, Texas, United States, 2018-10-09 - 2018-10-12. (LA-UR-18-29555)

Ganguly, K., R. C. Wiens, P. J. Gasda, R. T. Newell, A. L. Reyes-Newell, B. F. Sandoval, M. E. Dale, S. H. Adikari, C. D. Gleasner, S. J. Voit, C. Mensah, D. T. Seagraves, S. A. Wender, A. K. Misra, S. K. Sharma, H. M. Quinn, S. M. Clegg and S. Maurice. Benchmarking Organic Detection Limits with OrganiCam, for Remote Sensing from an Ocean World Lander or from a Mars Helicopter Mission. Presented at *AGU Fall Meeting 2020*, Zoom meeting, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29775)

Watkins, A. C. and H. M. Quinn. Evaluation of Electronic Performance in the Europa Environment. Presented at *20th Topical Meeting of the Radiation and Protection Shielding Division*, Santa Fe, New Mexico, United States, 2018-08-26 - 2018-08-26. (LA-UR-18-28218)

Posters

Wiens, R. C., P. J. Gasda, A. K. Misra, T. E. Acosta-Maeda, S. K. Sharma, H. M. Quinn, K. Ganguly, R. T. Newell, S. M. Clegg, S. Maurice, C. Virmontois, S. P. Love, A. E. Nelson, L. A. Ott and B. F. Sandoval. Organicam: A Lightweight Time-Resolved Fluorescence Imager and Raman Spectrometer for Organic Detection and Characterization. Presented at *LANL Engineering Week*, Los Alamos, NM, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21405)

Wiens, R. C., P. J. Gasda, A. Misra, T. Acosta-Maeda, S. Sharma, H. M. Quinn, K. Ganguly, S. P. Love, A. E. Nelson, R. T. Newell, S. M. Clegg, S. Maurice, C. Virmontois, L. A. Ott and B. F. Sandoval. Organicam: a lightweight time-resolved fluorescence imager and raman spectrometer for icy world organic detection and characterization. Presented at *50th LPSC*, The Woodlands, Texas, United States, 2019-03-18 - 2019-03-22. (LA-UR-19-22356)

Wiens, R. C., P. J. Gasda, H. M. Quinn, K. Ganguly, R. T. Newell, S. M. Clegg, S. P. Love, L. A. Ott, B. F. Sandoval, S. Maurice, C. Virmontois, A. K. Misra, T. E. Acosta-Maeda and S. K. Sharma. Organicam: A Lightweight Time-Resolved Fluorescence Imager and Raman Spectrometer for Organic Detection and Characterization. Presented at *American Geophysical Union Fall Conference*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32186)

Early Detection of Explosive Volcanic Eruptions Using Very High Frequency (VHF) Radiation from Vent Discharges

Sonja Behnke
20190107ER

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.

Publications

Journal Articles

Behnke, S. A., H. E. Edens, S. Senay, M. Iguchi and D. Miki. Radio Frequency Signal Characteristics of Volcanic Lightning. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-20-30282)

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)

Boron and Ribose in Clay: a Precursor for Life on Earth and Mars?

Patrick Gasda
20190238ER

Project Description

On Earth, there is a close association between life and the presence of clay minerals and boron. Clays and borates, separately, have been invoked as possible components for the origin of life on Earth. Our goal is to understand the signatures of boron-bearing clays so that they may be identified on Mars by rovers. If these signatures are identified on Mars, they will address one of the highest priority goals of the planetary science community: clear evidence of past or present microbial life on Mars.

Publications

Presentation Slides

Legett, S. A., C. M. Yeager, P. J. Gasda, M. A. Nellessen, L. Crossey, E. Peterson, N. L. Lanza, A. L. Reyes-Newell, D. M. Delapp, A. Labouriau, R. C. Wiens, S. M. Clegg and D. Das. Exploring potential origins of life on Earth and Mars by determining ribose stability in mixtures of borate-bearing clays. Presented at *Clay Minerals Society Annual Meeting*, Virtual, New Mexico, United States, 2020-10-19 - 2020-10-19. (LA-UR-20-28529)

Legett, S. A., C. M. Yeager, P. J. Gasda, M. Nellessen, L. Crossey, E. Peterson, N. L. Lanza, A. L. Reyes-Newell, D. M. Delapp, A. Labouriau, R. C. Wiens, S. M. Clegg and D. Das. Ribose Stability in Solutions with Borate and Borate-Bearing Clays: Implications for Origins of Life on Earth and Mars. Presented at *Lunar and Planetary Science Conference*, Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22277)

Posters

Nellessen, M., L. Crossey, P. J. Gasda, E. Peterson, N. L. Lanza, C. M. Yeager, A. Labouriau, R. C. Wiens and S. M. Clegg. Boron Adsorption In Clay Minerals: Implications For Martian Groundwater Chemistry And Prebiotic Processes. Presented at *Los Alamos Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26618)

Other

Nellessen, M. A., P. J. Gasda and L. Crossey. Boron Adsorption In Clay Minerals: Borate speciation modeling. Audio/Visual. (LA-UR-20-25598)

Reduced-profile Current-sheet Array (CSA) Antenna with Simpler Drive and Better Antenna Efficiency

MD Zuboraj
20190268ER

Project Description

The best antenna architecture for satellites today (the current-sheet array, or CSA) is not well suited for cubesat applications because the current CSA architecture has been optimized for ultra-high bandwidths (i.e., up to 900%) but not for compact size or aperture efficiency. Future cubesat-based national security missions will likely only need ~ 20% bandwidths, which allow us to reoptimize the CSA architecture with improved efficiency and smaller size. The impact of this technology development will be higher bandwidth communications on cubesats with greater directivity.

Publications

Posters

A. Zuboraj, M. R. and B. E. Carlsten. Beam-Current Loss in Emittance-Dominated High-Frequency Tubes. Presented at *IEEE Pulsed Power and Plasma Science Conference*, Orlando, Florida, United States, 2019-06-23 - 2019-06-28. (LA-UR-19-25558)

Quantum Metrology with an Atom Superconducting Quantum Interference Device (SQUID)

Changhyun Ryu
20190334ER

Project Description

Inertial sensing is essential in many critical national security missions. Although global positioning system (GPS)-based navigation can be used in ideal situations, when GPS service is denied or unavailable, an independent, accurate, inertial sensor is needed. Quantum metrology with an atom superconducting quantum interference device (SQUID) can increase the sensitivity in rotation sensing dramatically by utilizing macroscopic entanglement between angular momentum states. The successful completion of this project will demonstrate a revolutionary increase in rotation sensitivity from macroscopic entanglement. This will make it possible to develop a portable inertial sensor with the highest sensitivity for critical national security missions. This research is relevant to Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions of national security science in developing novel sensing technologies.

Publications

Journal Articles

*Ryu, C., E. C. Samson and M. G. Boshier. Quantum interference of currents in an atomtronic SQUID. 2020. *Nature Communications*. **11** (1): 3338. (LA-UR-20-25170 DOI: 10.1038/s41467-020-17185-6)

Presentation Slides

Ryu, C. Quantum Metrology with an Atom SQUID. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31465)

Novel, Fast Enhancements to Bragg Ptychography

Kevin Mertes
20190373ER

Project Description

The ability to rapidly produce non-destructive, three-dimensional (3D) images of crystalline nanostructures with nanometer resolution is directly relevant to our nation's national security. This research will provide a versatile tool that meets the needs of Department of Energy-Basic Energy Sciences, Weapons Science and Global Security Intelligence and Emerging Threats.

Publications

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)

Viral Mosaic Biosensor

Jessica Kubicek-Sutherland
20190392ER

Project Description

Influenza is a rapidly evolving viral pathogen that infects up to 5 million people annually. The early diagnosis and treatment of influenza infections can greatly reduce mortality. However, the currently available rapid influenza tests are unreliable and leave many infections undiagnosed. There is an urgent need for a highly sensitive influenza diagnostic test to be used in point-of-care settings. We will combine theoretical mosaic sequence design and the biosensor technology capabilities developed at Los Alamos National Laboratory to develop a rapid ultra-sensitive influenza biosensor using computationally-derived novel sequence probes that encompass a wide variety of influenza viruses to detect not only presently circulating viruses but potentially also future pandemic strains that will evolve through mutations and rearrangement. The resulting novel, inexpensive and highly sensitive diagnostic tool will be easily expandable to other pathogens, with influenza serving as a proof-of-principle. This work directly supports the Laboratory's Science of Signatures Pillar in threat reduction, biosurveillance and global health security and the missions of the DOE Office of Science Biological and Environmental Research (BER), as well as DHHS (NIH and CDC) missions to prevent, detect, diagnose, confront and treat disease, and is related to missions of DHS, DOD, and other federal agencies.

Publications

Journal Articles

Kubicek-Sutherland, J. Z., S. J. Courtney and Z. R. Stromberg. Nucleic Acid-Based Sensing Techniques for Diagnostics and Surveillance of Influenza. 2021. *Biosensors*. **11** (2): 47. (LA-UR-20-22835 DOI: 10.3390/bios11020047)

Stromberg, Z. R., J. P. Theiler, B. T. Foley, A. L. Myers y Gutierrez, A. D. Hollander, J. D. Gans, A. Deshpande, E. Martinez-Finley, H. Mukundan, K. Yusim and J. Z. Kubicek-Sutherland. Fast evaluation of viral emerging risks (FEVER) pipeline for detection and mutation typing of SARS-CoV-2. Submitted to *Nature Communications*. (LA-UR-21-21165)

Presentation Slides

Courtney, S. J. High-coverage diagnostic tool for SARS-like and influenza viruses. Presented at *Virtual interview presentation for University of Rochester PhD Program in Immunology, Microbiology, and Virology.*, Los Alamos, New Mexico, United States, 2021-02-05 - 2021-02-05. (LA-UR-21-20999)

Kubicek-Sutherland, J. Z. and S. J. Courtney. Beacons and Biosensors: An Approach to Influenza Diagnostics. . (LA-UR-20-25710)

Kubicek-Sutherland, J. Z. and Z. R. Stromberg. Investment Mentor Slides. . (LA-UR-20-23582)

Stromberg, Z. R. Development of SARS-CoV-2 RT-PCR Assays. . (LA-UR-20-29361)

Posters

Courtney, S. J., Z. R. Stromberg, J. P. Theiler, B. T. Foley, J. D. Gans, K. Yusim and J. Z. Kubicek-Sutherland. High-coverage nucleic acid probes for distinguishing SARS-CoV-2 from influenza. Presented at *Virtual Biophysical Society Annual Meeting 2021*, Los Alamos, New Mexico, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-20318)

Kubicek-Sutherland, J. Z., J. P. Theiler, K. Yusim, B. T. Foley, C. A. Lopez Bautista, S. Gnanakaran and H. Mukundan. Targeting Amphiphilic Biomarkers from Emerging Pathogens for Detection and Therapeutic Applications. Presented at *2019 Chemical and Biological Defense Science & Technology (CBD S&T) Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-31352)

Emulating Quantum Magnetism with Rydberg Atoms

Michael Martin
20190494ER

Project Description

The goal of this project to create a reconfigurable and tunable system for quantum emulation, based on dynamically-configurable arrays of individually-trapped ultracold rubidium atoms. The character, range and strength of the interaction between the atoms will be tuned by the geometry of the arrays, and by external laser parameters. This complete set of capabilities will be the first highly scalable, neutral atom-based platform for tackling a broad range of models in quantum magnetism. By exploring system behavior, such as spin correlations and ground states, we will improve understanding of important quantum many-body models. Further, we will study coherent quantum annealing as an approach to quantum optimization problems, which will inform ongoing research on the properties of commercially-available quantum devices, for which the exact role of entanglement and coherence is poorly understood. This work will impact basic understanding of materials, by elucidating the role of entanglement in material properties, such as the so-called quantum spin liquid ground state; information science/technology, by establishing a testbed for solving complex optimization problems through a process known as coherent quantum annealing; and advanced quantum sensing, where control over interactions yields robust quantum states for sensing beyond classical limits.

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)

Reports

Martin, M. J., M. C. Revelle and G. W. Biedermann. A platform for quantum information and large-scale entanglement with Rydberg atoms in programmable optical potentials. Unpublished report. (LA-UR-18-31881)

Presentation Slides

Martin, M. J. Emulating quantum magnetism with Rydberg atoms. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31519)

Martin, M. J. Emulating quantum magnetism with Rydberg atoms. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31484)

Martin, M. J. Neutral atom tools for quantum information science. Presented at *Meeting at Argonne Natl. Lab*, Lemont, Illinois, United States, 2019-03-25 - 2019-03-25. (LA-UR-19-22592)

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., C. Ryu and M. G. Boshier. Quantum technologies with ultracold atoms. Presented at *UC Quantum Information Science Research Workshop*, Berkeley, California, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24127)

de Melo, L. F. Past and Present Research in Atomic Physics. . (LA-UR-20-28126)

Discovering the 3D Structure and Dynamics of the Sun-Interstellar Medium System on a Global Scale

Daniel Reisenfeld
20190498ER

Project Description

The primary goal of this project is to understand the structure and dynamics of the Sun's space environment (the heliosphere) and its ability to screen the Earth from damaging radiation that is ubiquitous in the interstellar medium. Notably, this radiation, particularly cosmic rays, has a strong solar cycle variation; it also represents the greatest risk to interplanetary travel by humans as well as one of the largest backgrounds in National Nuclear Security Administration-sponsored, Los Alamos-built space instruments that detect nuclear explosions around the globe. The project exploits data from the Los Alamos-led energetic neutral atom (ENA) imager on the National Aeronautics Space Administration Interstellar Boundary Explorer (IBEX) mission to "sound" the three-dimensional extent of the heliosphere by monitoring over time the response of the outer heliosphere (via ENA emission) to bursts of plasma originally ejected from the Sun. By imaging the outer heliospheric response over time, we can understand the plasma flows and thus the underlying physical processes that govern heliospheric dynamics over the solar cycle. This research builds leadership capabilities in space weather and informs the optimization of the ENA imager that Los Alamos will lead for NASA's upcoming IMAP mission.

Publications

Journal Articles

*Reisenfeld, D. B., M. Bzowski, H. O. Funsten, P. H. Janzen, N. Karna, M. A. Kubiak, D. J. McComas, N. A. Schwadron and J. M. Sokol. The Influence of Polar Coronal Holes on the Polar ENA Flux Observed by IBEX. 2019. *Astrophysical Journal Letters*. **879** (1): 1. (LA-UR-19-22264 DOI: 10.3847/1538-4357/ab22c0)

Presentation Slides

Kim, K. H. Survey of Ion Properties in Jupiter's Plasma Sheet. Presented at *Juno MWG Team Meeting*, Los Alamos, New Mexico, United States, 2020-07-31 - 2020-07-31. (LA-UR-20-25669)

Reisenfeld, D. B. Sounding the Dimensions of the Heliosphere with IBEX. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-28330)

Posters

Reisenfeld, D. B., M. Bzowski, H. O. I. Funsten, J. Heerikhuisen, P. Janzen, M. A. Kubiak, D. J. McComas, N. A. Schwadron, J. Sokol and E. Zirnstein. Building a 3-D Map of the Heliosphere with IBEX. Presented at *2020 Fall Meeting of the American Geophysical Union*, San Francisco, California, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29579)

Reisenfeld, D. B., M. Bzowski, H. O. I. Funsten, P. H. Janzen, M. A. Kubiak, D. J. McComas, N. A. Schwadron and J. Sokol. Sounding The Dimensions of the Heliosphere Using the Time-Correlation Between IBEX ENA Observations and the Solar Wind Dynamic Pressure. Presented at *2019 Fall Meeting of the American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-32234)

Rare Earth Fission Product Element Separations by High Speed Counter-Current Chromatography

Iain May
20200116ER

Project Description

The rare earths are a series of elements that have very similar chemical properties, rendering their separation and purification extremely challenging. The analysis of radioactive rare earth elements adds significantly to this challenge. Our goal to to apply novel separation technology to significantly improve our ability to produce chemically and radiochemically pure samples. The separation and purification of rare earth elements supports multiple nuclear security and energy security missions.

Gossamer Radio Frequency (RF) Satellite Parabola Made by Additive Manufacturing

Jeremiah Rushton
20200180ER

Project Description

This project will enhance the capability of orbital space assets. Its novel way to make a large dish for a compact satellite communication will be greatly disruptive for small-to-medium sized space assets. It is much more compact than any current technology and when developed will allow more agile design, faster design and rapid deployment of space assets for Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions dovetailing with other agencies. The patent-pending concept is simple; assemble a dish in orbit from compact, lightweight components.

Unveiling the Heating and Acceleration of Solar Wind by “Touching” the Sun with the Parker Solar Probe

John Steinberg
20200270ER

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.

Publications

Journal Articles

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

*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)

Li, H. Fast Magnetic Reconnection with Turbulence in High Lundquist Number Limit. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-24765)

*Seo, B., P. Wongwaitayakornkul, M. A. Haw, R. S. Marshall, H. Li and P. M. Bellan. Determination of a macro- to micro-scale progression leading to a magnetized plasma disruption. 2020. *Physics of Plasmas*. **27** (2): 22109. (LA-UR-20-28589 DOI: 10.1063/1.5140348)

Presentation Slides

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. and X. Fu. Heating of Heavy Ions in Low-beta Compressible Turbulence. Presented at *2019 AGU Fall Meeting*, san francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-20-28060)

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)

Deep Learning Interferometric Synthetic-Aperture Radar

Bertrand Rouet-Leduc
20200278ER

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.

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)

*Rouet-Leduc, B., C. Hulbert, I. W. McBrearty and P. A. Johnson. Probing Slow Earthquakes With Deep Learning. 2020. *Geophysical Research Letters*. **47** (4). (LA-UR-19-27444 DOI: 10.1029/2019GL085870)

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)

The Role of Defects in Solid State Detonation Kinetics

Pamela Bowlan
20200311ER

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.

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)

Presentation Slides

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)

Parallel Magnetic Resonance Imaging with a Multichannel Radio-frequency Atomic Magnetometer

Young Jin Kim
20200393ER

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.

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. M. and Y. J. Kim. Investigation of magnetic noise from conductive shields in the 10–300 kHzfrequency range. Submitted to *Journal of Applied Physics*. (LA-UR-20-27307)

Presentation Slides

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)

Posters

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)

Broadband Terahertz Circular Dichroism Spectroscopy

Houtong Chen
20200419ER

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.

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., 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)

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)

High Energy Lightning: Understanding Relations Between Energetic Particles and Lightning Discharges in Thunderclouds

Xuan-Min Shao
20170179ER

Project Description

This project directly addresses Department of Energy(DOE)/National Nuclear Security Administration(NNSA) space-based nuclear detonation detection missions, as well as the nation's newly developed ground-based nuclear forensics missions. Lightning-related electromagnetic pulse (EMP) and gamma/x-ray emission signatures are often similar to those of atmospheric nuclear explosions and are unwanted background interference for these systems. Better understanding of their signatures and the underlying physics is important to reducing the possible false alarms for these systems. Los Alamos National Laboratory's ground-based EMP observation and advanced simulation play a critical role in providing prompt nuclear weapon performance information for a national-level forensics mission. However, without actual nuclear tests it is difficult to validate the sensor and the simulation performance. Fortunately, EMP and gamma emissions produced by cosmic ray showers and lightning are similar (in a small scale) in physics to that of a nuclear explosion, especially at the exponential multiplication stage, and can be used to validate the United States Prompt Detection System (USPDS) sensor and simulation.

Technical Outcomes

The project developed the world’s first Broadband Interferometric Mapping and Polarization (BIMAP) system for lightning physics study. BIMAP observations, in conjunction with theoretical modeling, revealed a number of new physics in lightning processes, including lightning initiation that is apparently ignited by cosmic-ray showers (CRS). The team also detected “gamma glow” and discovered it is due to modification of CRS in a thunderstorm’s electric field. First observations of spectrum-resolved neutron bursts found that they are due to CRS interactions with soil materials.

Publications

Journal Articles

*Bowers, G. S., W. Blaine, X. Shao, B. Dingus, D. M. Smith, M. Schneider, F. Martinez-McKinney, M. P. McCarthy, S. BenZvi, L. Nellen and N. Fraija. Combining Cherenkov and scintillation detector observations with simulations to deduce the nature of high-energy radiation excesses during thunderstorms. 2019. *Physical Review D*. **100** (4): 043021. (LA-UR-19-25406 DOI: 10.1103/PhysRevD.100.043021)

Bowers, G. S., X. Shao, W. G. Blaine, B. L. Dingus, D. M. Smith, J. Chaffin, J. Ortberg, H. K. Rassoul, C. Ho, L. Nellen and N. Fraija. Spectral Characteristics of Neutron Bursts by Cosmic Ray Showers and Implications for Terrestrial Gamma-ray Flash (TGF) Signatures. Submitted to *Geophysical Research Letters*. (LA-UR-20-22967)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine and B. L. Dingus. Improving RF Lightning Mapping Accuracy with “Focused” Interferometry. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-19-24094)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine and B. L. Dingus. “Focused Interferometry” and Fine Structure of Lightning-Initiating Fast Positive Streamers. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-19-32549)

*Shao, X., C. Ho, M. Caffrey, P. Graham, B. Haynes, G. Bowers, W. Blaine, B. Dingus, D. Smith and H. Rassoul. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations of Lightning Discharges: Revealing New Physics Insights Into Breakdown Processes. 2019. *Journal of Geophysical Research: Atmospheres*. **123** (18): 10-10. (LA-UR-18-24675 DOI: 10.1029/2018JD029096)

Conference Papers

Bowers, G. S., X. Shao, W. G. Blaine, B. L. Dingus, D. M. Smith, M. Schneider and M. McCarthy. Simulation of the High Altitude Water Cherenkov (HAWC) Observatory & Gamma-ray Observations During Overhead Thunderstorms (GODOT) instrument to Relativistic Runaway Electron Avalanche (RREA) gamma-ray enhancements. Presented at *16th International Conference on Atmospheric Electricity (ICAE)*. (Nara, Japan, 2018-06-17 - 2018-06-22). (LA-UR-18-23454)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine, B. L. Dingus, M. P. Caffrey, P. S. Graham, W. B. Haynes and D. Smith. Broadband RF interferometric and polarization observations of lightning discharges correlated with gamma flux detection. Presented at *XVI International Conference on Atmospheric Electricity*. (Nara, Japan, 2018-06-17 - 2018-06-22). (LA-UR-18-23483)

Presentation Slides

Bowers, G. S., D. M. Smith, M. P. McCarthy, J. R. Dwyer, X. Shao and B. L. Dingus. Gamma-ray Signatures of Neutrons from Terrestrial Gamma-ray Flahses. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31117)

Bowers, G. S., W. G. Blaine, X. Shao, B. L. Dingus, M. P. McCarthy, M. Schneider, J. Chaffi and D. Smith. HAWC & GODOT Observation of Thunderstorm Ground Enhancements. Presented at *American Geophysical Union 2018*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31303)

Bowers, G. S. and D. M. Smith. Neutrons From Terrestrial Gamma-ray Flashes. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31120)

Bowers, G. S. and X. Shao. Understanding Electromagnetic Pulse & Energetic Particle Signatures from Lightning. Presented at *Interagency Technical Nuclear Forensics Technical Overview (ITNFTR)*, Oak Ridge, Tennessee, United States, 2018-06-30 - 2018-06-30. (LA-UR-18-25311)

Shao, X. Ionosphere disturbances introduced by thunderstorms and lightning discharges. Presented at *International Symposium on Lightning Physics and Lightning Meteorology*, Beijing, China, 2017-09-24 - 2017-09-27. (LA-UR-17-28257)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine, B. L. Dingus, M. P. Caffrey, P. S. Graham, W. B. Haynes, D. Smith and H. Rassoul. Broadband RF interferometric and polarization observations of lightning discharges correlated with gamma flux detection. Presented at *16th International Conference on Atmospheric Electricity*, Nara, Japan, 2018-06-17 - 2018-06-22. (LA-UR-18-25227)

Shao, X., C. Ho, M. P. Caffrey, P. S. Graham, W. B. Haynes, B. L. Dingus and G. S. Bowers. Broadband RF Interferometric and Polarization Observations of Lightning Discharge Processes. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-30958)

Shao, X., G. S. Bowers, C. Ho, B. L. Dingus, J. S. Bull and C. S. Meierbachtol. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations Reveal new Physics Insights into Lightning Discharge Processes. Presented at *American Geophysical Union Fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31981)

Shao, X., G. S. Bowers, W. G. Blaine, C. Ho and B. L. Dingus. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations of Mini-Discharges in Thunderstorms. Presented at *American Geophysical Union Fall meeting, 2018*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31298)

Shao, X., J. S. Bull and C. S. Meierbachtol. Signatures of RF Polarization Related to Relativistic Discharge Processes. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31977)

Posters

Blaine, W. G., G. S. Bowers, X. Shao and B. L. Dingus. Simulating Electric Field Effects on Cosmic Ray Particle and Radio Frequency Observations. Presented at *American Geophysical Union (AGU) Fall Meeting 2018*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31431)

Other

Shao, X. Data for “Lightning Interferometry Uncertainty, “Focused Interferometry”, and Evidence of Lightning being Ignited by a Cosmic-ray Shower” by Shao et al.. Dataset. (LA-UR-20-22794)

Atomic Structure of Actinides

Igor Savukov
20180125ER

Project Description

Knowledge of the properties of actinide atoms is central to Los Alamos National Laboratory mission applications. In particular, atomic properties, such as energy levels and transition rates, are needed for spectroscopy-based applications, such as detection of actinide atoms and enrichment characterization, and for plasma modeling. Currently, there are no theories adequate for this task. This project will develop an accurate atomic structure theory that will be capable of generating data needed in various applications.

Technical Outcomes

Atomic theory has been developed for applications in complex atoms, especially actindies. Among theoretical approaches, a parametric configuration-interaction many-body perturbation theory was selected and developed. Various properties were calculated in agreement with experiment. The theory was applied to atomic property calculations for various applications, such as plasma modeling, development of propulsion systems and bright sources for lithography, astrophysics, and actinide spectroscopy. The new atomic structure capability was used in support of Laboratory mission relevant applications.

Publications

Journal Articles

*Filin, D., I. M. Savukov and J. Colgan. CI-MBPT line strengths and atomic probabilities for some transitions of neutral iodine. 2020. *Journal of Physics B: Atomic, Molecular and Optical Physics*. **53** (14): 145003. (LA-UR-20-20076 DOI: 10.1088/1361-6455/ab8c57)

Filin, D. and I. M. Savukov. Accurate CI-MBPT calculation of radiative lifetimes and transition probabilities of neutral lanthanum (La I) odd states with J = 3/2. 2020. *Physica Scripta*. **95** (10): 105401. (LA-UR-20-23523 DOI: 10.1088/1402-4896/abb421)

Savukov, I. M. CI-MBPT and intensity-based lifetime calculations for Th II. Submitted to *MDPI*. (LA-UR-20-28610)

*Savukov, I. M. and P. M. Anisimov. Configuration-interaction many-body perturbation theory for La ii electric-dipole transition probabilities. 2019. *Physical Review A*. **99** (3): 032507. (LA-UR-18-30155 DOI: 10.1103/PhysRevA.99.032507)

Presentation Slides

Filin, D., I. M. Savukov and J. P. Colgan. Accurate CI-MBPT calculation of radiative lifetimes and transition probabilities of neutral lanthanum (La I). Presented at *51st Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Portland, Oregon, United States, 2020-06-01 - 2020-06-05. (LA-UR-20-24070)

Savukov, I. M. Application of many-body perturbation theory to actinide atoms. Presented at *Atomic Physics 2018*, Boston, Massachusetts, United States, 2018-10-26 - 2018-10-27. (LA-UR-18-29977)

Savukov, I. M. Ab initio precision CI-MBPT calculations for noble-gas atoms. Presented at *Atomic Physics 2018*, Boston, Massachusetts, United States, 2018-10-26 - 2018-10-27. (LA-UR-18-30184)

Savukov, I. M. Accurate calculations of La II transition probabilities with CI-MBPT method. Presented at *ICAMDATA-2018*, Cambridge, Massachusetts, United States, 2018-11-11 - 2018-11-15. (LA-UR-18-30699)

Savukov, I. M. Atomic structure calculations of complex atoms: review. . (LA-UR-19-23852)

Savukov, I. M. CI-MBPT calculations of energies, transitions, and g factors of La II and La I. Presented at *50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Milwaukee, Illinois, United States, 2019-05-27 - 2019-05-27. (LA-UR-19-24759)

Posters

Filin, D., I. M. Savukov and J. P. Colgan. CI- MBPT calculations of the iodine line strengths. Presented at *DAMOP*, Milwaukee, Wisconsin, United States, 2019-05-27 - 2019-05-31. (LA-UR-19-24863)

Filin, D., I. M. Savukov and J. P. Colgan. Accurate CI-MBPT calculation of radiative lifetimes and transition probabilities of neutral lanthanum (La I). Presented at *51st Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Portland, Oregon, United States, 2020-06-01 - 2020-06-05. (LA-UR-20-23994)

Filin, D., J. P. Colgan and I. M. Savukov. Ab Initio CI-MBPT Energy Levels and Line Strengths of the Sn XIII-Sn XVI Ions for 13-14 nm Lithography. Presented at *International Conference on Numerical Simulation of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28863)

Active Sensing for Short-Range Remote Detection and Characterization

Ann Ollila
20200614ER

Project Description

Laboratory missions that use optical remote sensing of key chemical and physical quantities include nonproliferation, counter-proliferation, and planetary science. These missions benefit greatly when new signatures and sensing techniques provide additional information not previously available. Research in passive remote optical spectroscopy has been conducted for decades at Los Alamos, with very large investments over that time. As a result of these efforts, Los Alamos has become a world leader in stand-off analyses for planetary science and other purposes. To complement these existing investments, this proposal concentrates on active optical and acoustic remote sensing. The development of the SuperCam instrument for the National Aeronautics Space Administration (NASA) Mars 2020 rover mission provides the team with the basic instrumentation and analysis tools to perform that mission. However, broader application of these technologies to national-security and other science missions requires a deeper understanding of the science underlying the observed signatures and variations of the sensing methods used for SuperCam. The proposed research will build a foundation for future instruments to be used in nuclear safeguards and homeland security.

Technical Outcomes

This project took a multi-pronged approach to advance remote spectral techniques including Laser-induced Breakdown Spectroscopy (LIBS), Time-Resolved Luminescence Spectroscopy (TRLS), Raman spectroscopy, LIBS acoustics, and reflectance spectroscopy. The team studied the development of instrument response functions and collected luminescence spectra of trace elements in minerals. The team also developed a sample suite of varying grain sizes to study the effects on Raman signals and developed a new methodology for creating artificial coatings on rocks for studies of LIBS acoustics.

High Efficiency Active Environmental Sampling of Chemical Traces

Sylvia Ann Junghans
20190517ECR

Project Description

The proposed work aims to deliver an active sampling matrix that enhances the Raman signature of a target analyte thereby enabling in-field analysis by handheld instruments. Successful completion of the proposed work could result in a disruptively new detection method for fast in-field analysis of traces of a multitude of Raman active chemicals (e.g. high explosives, hazardous chemicals, chemical and biological warfare agents) relevant for national security applications.

Publications

Posters

Junghans, S. A., S. Bajric, L. E. Wolfsberg, E. S. Davis, C. Pantea, G. S. Goff, B. L. Scott, R. E. Lakis and V. Henzl. High Efficiency Active Environmental Sampling of Chemical Traces. Presented at *LANL Global Security Symposium*, Los Alamos, New Mexico, United States, 2019-11-13 - 2019-11-13. (LA-UR-19-31344)

Granddaughter Radiochronometry for Nuclear Forensics

Joanna Denton
20190565ECR

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.

Publications

Presentation Slides

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)

Understanding the Wave Mechanics of Micro-architected Waveguides to Design Acoustic Quick Response Codes

Vamshi Chillara
20190568ECR

Project Description

This project develops a first of its kind acoustic Quick Response (QR) code system that can store information in the acoustic wave response characteristics of structures. Acoustic QR codes do not broadcast information and cannot be tampered/intruded/compromised with any existing wireless technologies. Thus, they can provide an additional layer of security for applications in nuclear proliferation and global security. The outcomes of this research effort will have applications in chemical/ biomaterials characterization and energy security.

Publications

Journal Articles

Chillara, V., C. N. Hakoda and C. Pantea. On the in-plane vibrations and electromechanical resonance characteristics of non-uniformly polarized rectangular piezoelectric wafers: selective mode-type excitation and specific mode enhancement. Submitted to *Journal of Sound and Vibration*. (LA-UR-20-26559)

Chillara, V., J. J. Greenhall, C. N. Hakoda and C. Pantea. Does the electromechanical impedance spectrum always show mechanical resonances of a piezoelectric wafer?. Submitted to *Ultrasonics*. (LA-UR-20-30362)

Chillara, V., J. J. Greenhall and C. Pantea. Ultrasonic waves from radial mode excitation of a piezoelectric disc on the surface of an elastic solid. Submitted to *Ultrasonics*. (LA-UR-19-27754)

Hakoda, C. N., E. S. Davis, C. Pantea and V. Chillara. Piezoelectric Quick Response (PQR) codes with multi-level information storage. Submitted to *Physical Review Applied*. (LA-UR-20-23220)

Hakoda, C. N., V. Chillara and C. Pantea. The Effect of a Transducer’s Spatial Averaging on an Elastodynamic Guided Wave’s Wavenumber Spectrum. Submitted to *Ultrasonics*. (LA-UR-20-25258)

Conference Papers

Hakoda, C. N., C. Pantea and V. Chillara. Investigation of resonance enhancement through non-uniform piezoelectric polarization for information storage methodology. Presented at *SPIE Smart Structures + NDE 2020 - New Digital Forum*. (Anaheim, California, United States, 2020-04-26 - 2020-04-30). (LA-UR-20-22867)

Presentation Slides

Chillara, V. Non-traditional information storage using acoustics and vibrations. . (LA-UR-20-27431)

Hakoda, C. N., C. Pantea and V. Chillara. Engineering the quasi-Rayleigh wave's beat phenomenon for embedded information storage. . (LA-UR-20-25201)

Posters

Hakoda, C. N., C. Pantea and V. Chillara. Investigation into form factors for mechanical-resonance-based methods of information storage. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21738)

Hakoda, C. N., C. Pantea and V. Chillara. Engineering the quasi-Rayleigh wave's beat phenomenon for embedded information storage. Presented at *IEEE International Ultrasonics Symposium*, Los Vegas, Nebraska, United States, 2020-09-06 - 2020-09-11. (LA-UR-20-26656)

In-Process, Full Part Defect Detection for Additive Manufacturing

Adam Wachtor
20190580ECR

Project Description

This work supports the national security mission by improving the capability to produce mission-critical parts through additive manufacturing. Additive manufacturing allows for the production of unique components without the need for significant preparation and tooling costs seen in traditional fabrication processes. These advances in non-destructive evaluation for in-process additive manufacturing may lead to active feedback and control of the additive manufacturing process and benefit quality control and part certification. This in turn will allow for the production of reliable components in-house that support stockpile life-extension programs and retrofits and provide low-cost handling and tooling fixtures for fabrication services.

Publications

Journal Articles

Eckels, J. D., E. M. Jacobson, I. T. Cummings, I. F. Fernandez, K. Ho, N. Dervilis, E. B. Flynn and A. J. Wachtor. Predicting Local Material Thickness from Steady-State Ultrasonic Wavefield Measurements Using a Convolutional Neural Network. Submitted to *NDT & E International*. (LA-UR-21-21310)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, N. Calta, G. Guss, J. Forien, M. Matthews and P. Depond. In-Situ Process Monitoring of Laser Sintering via Classification of Acoustic Emissions. Submitted to *Additive Manufacturing*. (LA-UR-20-26003)

Tempelman, J. R., M. K. Mudunuru, S. Karra, A. J. Wachtor, E. B. Flynn, B. Ahmmed, J. Forien, G. Guss, M. Matthews, P. Depond and N. Calta. Machine Learning to Discover Pore Formation Signatures and Predict Pore Location during Additive Manufacturing Process. Submitted to *Additive Manufacturing*. (LA-UR-20-26174)

Conference Papers

Cummings, I. T., E. M. Jacobson, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. IN-PROCESS DEFECT DETECTION FOR ADDITIVELY MANUFACTURED METAL LATTICES. Presented at *IMECE\xc2\xae International Mechanical Engineering Congress & Exposition*. (Portland, Oregon, United States, 2020-11-15 - 2020-11-19). (LA-UR-20-23494)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. Defect Detection in Additively Manufactured Metal Parts Using In-Situ Steady-State Ultrasonic Response Data. Presented at *International Mechanical Engineering Congress & Exposition*. (Portland, Oregon, United States, 2020-11-13 - 2020-11-18). (LA-UR-20-23495)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. DEFECT DETECTION IN ADDITIVELY MANUFACTURED METAL PARTS USING IN-SITU STEADY-STATE ULTRASONIC RESPONSE DATA. Presented at *International Mechanical Engineering Congress & Exposition (IMECE)*. (Portland, Oregon, United States, 2020-11-13 - 2020-11-13). (LA-UR-20-25128)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. Using Steady-State Ultrasonic Direct-Part Measurements for Defect Detection in Additively Manufactured Metal Parts. Presented at *International Modal Analysis Conference (IMAC)*. (Virtual, New Mexico, United States, 2021-02-08 - 2021-02-11). (LA-UR-20-30178)

Presentation Slides

Cummings, I. T., E. M. Jacobson, A. J. Wachtor and E. B. Flynn. Acoustic Steady-State-Excitation Spatial Spectroscopy (ASSESS). Presented at *DisrupTECH Texas A&M Design Sprint Workshop*, Online, New Mexico, United States, 2021-02-24 - 2021-02-26. (LA-UR-21-21542)

Cummings, I. T., E. M. Jacobson, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. In-Process Defect Detection for Additively Manufactured Metal Lattices. Presented at *ASME International Mechanical Engineering Congress & Exposition 2020*, Online, New Mexico, United States, 2020-11-16 - 2020-11-19. (LA-UR-20-27464)

Jacobson, E. M., I. T. Cummings, E. B. Flynn and A. J. Wachtor. In-Situ Direct Inspection of Additively Manufactured Metal Parts. Presented at *Engineer's Week*, Los Alamos, New Mexico, United States, 2021-02-22 - 2021-02-25. (LA-UR-21-21603)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, A. J. Wachtor and E. B. Flynn. IMECE 2020 Video Presentation Script and Abstract. Presented at *ASME IMECE 2020*, Portland, Oregon, United States, 2020-11-16 - 2020-11-19. (LA-UR-20-27467)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. IMAC XXXIX 10532: Using Steady-State Ultrasonic Direct-Part Measurements for Defect Detection in Metal Additively Manufactured Parts. Presented at *IMAC XXXIX*, Online, New Mexico, United States, 2021-02-08 - 2021-02-11. (LA-UR-20-30509)

Mellos, G. N., P. H. Fickenwirth, C. J. Montgomery, A. J. Wachtor and E. B. Flynn. Estimating Porosity of AM Constructed 304L SS Cylinders Using Process Parameters. . (LA-UR-19-26285)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, G. Guss, J. Forien, N. Calta and M. Matthews. In-Situ Process Monitoring for Defect Prediction in Laser Powder Bed Fusion. Presented at *Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-25. (LA-UR-20-21832)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Feature Extraction of Acoustic Emissions. . (LA-UR-19-26291)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Sensor Fusion for Keyhole Identification in Laser Powder-bed Fusion Additive Manufacturing. Presented at *Los Alamos Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25464)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Updates on LANL AM Data Analysis. . (LA-UR-20-25768)

Wachtor, A. J. In-Process Quality Control of Additively Manufactured Parts. . (LA-UR-19-21711)

Wachtor, A. J., J. R. Tempelman, E. B. Flynn, G. Guss, J. Forien, N. Calta and M. Matthews. In-Situ Acoustic Monitoring of Metal Powder Bed Fusion Processes. Presented at *Cross-JOWOG on AM*, Livermore, California, United States, 2020-01-27 - 2020-01-27. (LA-CP-20-20093)

Posters

Fickenwirth, P. H., C. J. Montgomery, E. B. Flynn and A. J. Wachtor. In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27760)

Jacobson, E. M., P. H. Fickenwirth, A. J. Wachtor and E. B. Flynn. Damage Detection in Metallic Additively Manufactured Parts using In-Situ Steady-State Ultrasonic Response Data. Presented at *LANL Engineer's Week 2020*, Los Alamos, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21545)

Mellos, G. N., P. H. Fickenwirth, C. J. Montgomery, E. B. Flynn and A. J. Wachtor. In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing. Presented at *LANL E-Week Poster Session*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-20. (LA-UR-19-21306)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. . (LA-UR-19-27835)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. . (LA-UR-19-27862)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. Presented at *Solid Free form Fabrication*, Austin, Texas, United States, 2019-08-12 - 2019-08-15. (LA-UR-19-28147)

Using Thundercloud Illumination by Lightning to Understand Optical Signal Propagation in Nature

Michael Peterson
20200529ECR

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.

Publications

Journal Articles

Peterson, M. J. Holes in Optical Lightning Flashes: Identifying Poorly-Transmissive Clouds in Lightning Imager Data. 2020. *Earth and Space Science*. (LA-UR-20-22888 DOI: 10.1029/2020EA001294)

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. Modeling the Transmission of Optical Lightning Signals Through Complex 3-D Cloud Scenes. 2020. *Journal of Geophysical Research: Atmospheres*. **125** (23). (LA-UR-20-23479 DOI: 10.1029/2020JD033231)

Peterson, M. J. The Illumination of Thunderclouds by Lightning: Part 1: The Extent and Altitude of Optical Lightning Sources. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-21-22307)

Peterson, M. J. The Illumination of Thunderclouds by Lightning: Part 2: The Effect of GLM Instrument Threshold on Detection and Clustering. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-21-22572)

Peterson, M. J. and G. Stano. The Hazards Posed by Mesoscale Lightning Megaflashes. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-20-25866)

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)

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)

Understanding Optical Signatures from Natural and Artificial Aurora

Rebecca Sandoval
20200555ECR

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)

Nitrogen: Abundant on Earth and Forgotten in Space

Philip Fernandes
20200580ECR

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.

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)

Geospatial Change Surveillance with Heterogeneous Data

Amanda Ziemann
20180529ECR

Project Description

The work in this project enables the development and application of meaningful geospatial change detection from heterogeneous satellite data streams. This is a longstanding challenge in the science and national security communities, as identified by the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) and National Geospatial-Intelligence Agency (NGA). The capability developed in this project will leverage multiple satellite sensors, and integrate them across time to surveil particular areas. The case study is the detection of Siberian methane craters through a sophisticated change surveillance approach, and the understanding of these craters is important as they have significant climate implications. The methane craters serve as a proxy for nonproliferation and proliferation detection applications. The expected outcome is a capability that can ingest a constant stream of multi-sensor satellite imagery for a targeted area of interest, and perform both automated cueing and broad area search.

Publications

Journal Articles

Ren, C. X., A. Ziemann, J. P. Theiler and A. Durieux. Cycle-Consistent Adversarial Networks for Realistic Pervasive Change Generation in Remote Sensing Imagery. Submitted to *Proceedings of the IEEE arXiv*. (LA-UR-19-31936)

*Theiler, J., A. Ziemann, S. Matteoli and M. Diani. Spectral Variability of Remotely Sensed Target Materials: Causes, Models, and Strategies for Mitigation and Robust Exploitation. 2019. *IEEE Geoscience and Remote Sensing Magazine*. **7** (2): 8-30. (LA-UR-19-25129 DOI: 10.1109/MGRS.2019.2890997)

Ziemann, A., C. X. Ren and J. P. Theiler. Multi-sensor anomalous change detection at scale. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-19-24295)

Conference Papers

Theiler, J. P., M. Kucer and A. Ziemann. Experiments in Anomalous Change Detection with the Viareggio 2013 Trial Dataset. Presented at *SPIE Defense+Commercial Sensing*. (Anaheim (VIRTUAL), California, United States, 2020-04-27 - 2020-04-30). (LA-UR-20-23618)

Theiler, J. P. and A. Ziemann. Background estimation in multispectral imagery. Presented at *OSA Hyperspectral Imaging and Sounding of the Environment*. (San Jose, California, United States, 2019-06-25 - 2019-06-27). (LA-UR-19-21593)

Books/Chapters

Ziemann, A. and S. Matteoli. Detection of Anomalous and Large-Scale Changes. (LA-UR-19-23173)

Ziemann, A. and S. Matteoli. Detection of Large-Scale and Anomalous Changes. (LA-UR-19-23681)

Presentation Slides

Ren, C. X., A. Ziemann, A. Durieux and J. P. Theiler. Cycle-Consistent Adversarial Networks for Realistic Pervasive Change Generation in Remote Sensing Imagery. Presented at *Southwest Symposium on Image Analysis and Interpretation*, Santa Fe, New Mexico, United States, 2020-03-30 - 2020-03-30. (LA-UR-20-22555)

Theiler, J. P. Machine Learning for Background Estimation in Multispectral Imagery. . (LA-UR-18-30337)

Theiler, J. P. Finding the undefined: anomalous signals in cluttered backgrounds. Presented at *Southwest Symposium on Image Analysis and Interpretation*, Santa Fe, New Mexico, United States, 2020-03-30 - 2020-03-31. (LA-UR-20-22599)

Theiler, J. P., A. Ziemann and M. Kucer. Experiments in anomalous change detection with the Viareggio dataset. Presented at *SPIE Defense + Commercial Sensing*, Anaheim, California, United States, 2020-04-26 - 2020-04-30. (LA-UR-20-22859)

Ziemann, A., C. X. Ren and J. P. Theiler. Multi-Sensor Anomalous Change Detection at Scale. . (LA-UR-19-23682)

Ziemann, A., G. Fairchild, J. R. Conrad, C. A. Manore, N. K. Parikh, S. Y. Del Valle and E. N. A. Generous. Predicting dengue incidence in Brazil using broad-scale spectral remote sensing imagery. Presented at

International Geoscience and Remote Sensing Symposium (IGARSS), Valencia, Spain, 2018-07-22 - 2018-07-27. (LA-UR-18-26809)

Ziemann, A., J. P. Theiler, C. X. Ren and M. Kucer. Physics-based machine learning for detecting changes and targets in spectral imagery. . (LA-UR-20-23541)

Science of Signatures

Early Career Research
Final Report

Establishing a Scientific Understanding for the Generation of Radiofrequency Signals from High Explosives

Kendra Van Buren
20180589ECR

Project Description

Radio-frequency (RF) measurements offer the potential to diagnose properties of high explosives (HE) during detonation. Despite the wealth of experimental results published in the last three decades, no predictive capability of RF production currently exists because the theoretical understanding of how intrinsic properties (density, composition, porosity, piezoelectric content, etc.) of HE might contribute to RF production is to a great extent incomplete. This research project will help to close this gap through a combination of experiments, signal processing, and simulation capability to explore the extent to which RF emissions can be used to reliably assess HE detonation. Establishing a scientific understanding of HE properties that contribute to RF emissions will stimulate its reliable use as a novel diagnostic for hydrodynamic testing. This, in turn, offers the potential to yield novel metrics for the validation of both HE models and integrated simulations. It will also set the stage to implement computational models of RF generation, which are currently not available in Advanced Scientific Computing (ASC) codes.

Technical Outcomes

This LDRD project successfully carried out experiments that tried to isolate different factors that could potentially lead to the generation of signatures in radio-frequency signals. The experiments were unable to observe appreciable differences between the plastic bonded explosive (PBX)-9501 and diaminoazoxyfurazan (DAAF) or when the density of high explosive (HE) is varied. It is possible that the variations explored were too small to create observable differences. However, the team was able to observe repeatable signatures from the detonators and other features in experiments.

Publications

Presentation Slides

Johnson, C. E., K. L. Van Buren, H. R. J. Anaya, L. J. Lynch, J. F. Vigil, E. J. Salazar and F. M. Hemez. Detonation Electric Effect Measurements in PBX 9501 and Comparison with Hydrocode Calculations. Presented at *APS SCCM 2019*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25524)

Tracking Ultrafast Morphology Changes in Solid Explosives During a Detonation using Visible Laser Speckle

Pamela Bowlan
20180597ECR

Project Description

Our weapons stockpile relies entirely on a small number of secondary high explosive materials, such as octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Energetic materials exhibit a unique and complex interplay of shock physics, chemistry, kinetics and thermodynamics, giving rise to the highly coherent phenomenon of detonation. Even after decades of research there are still significant uncertainties in our ability to predict and control when and how energetic materials release energy, which has serious implications for safety and performance of explosives. One reason is that, while chemical kinetics are understood in gases and liquids, much less is known about how reactions proceed within a crystalline lattice. Secondly, events like detonation, where a bulk material can go from ambient conditions to pressures of Gigapascals (GPa) and temperatures of ~ 4000 kelvin (K) within a nanosecond (ns) are extremely difficult to measure. While studying explosives with visible lasers has been avoided in the past since they are highly scattering powders, our innovation is to use the resulting laser speckle as an instantaneous probe of a material's morphology during detonation. This technique will reveal important basic science facts missing from current models about how the extreme temperatures and pressures which lead to detonation are generated in explosive materials.

Technical Outcomes

The project introduced a new method of probing ultrafast changes in phase and density and applied this to learn more about what a detonation wave is and why some solid explosives are more sensitive than others. This method should be applicable to other measurements of materials in extreme conditions where it is necessary to time resolve phase and density changes. The team transitioned the application of this method in impact experiments as part of a new Joint Munitions Program project.

Publications

Conference Papers

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius, N. A. Suvorova and D. M. Oschwald. Resolving the loss of crystallinity during a detonation with visible light scattering. Presented at *The APS topical meeting on Shock Compression of Condensed Matter*. (Portland, Oregon, United States, 2019-06-17 - 2019-06-17). (LA-UR-19-27100)

Presentation Slides

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius, N. A. Suvorova and D. M. (. Oschwald. Time resolving the loss of crystallinity during detonation in a secondary solid explosive. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21854)

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius, N. A. Suvorova and D. M. Oschwald. Resolving the ultrafast loss of crystallinity during a detonation with visible light scattering. Presented at *Shock Compression of Condensed Matter*, portland, Oregon, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25369)

Persistent Signatures of Neutron Fluence in Structural Materials

Anthony Pollington
20190595ECR

Project Description

To this date, all nuclear weapons states including the United States of America have followed relatively similar paths to achieving a working arsenal. One of the steps that is common to all known nuclear weapons programs is the testing of material in criticality experiments. These experiments impart chemical signatures on the material around them (concrete, dirt, steel, etc.), which can potentially be measured and can be used to infer what types of activities occurred. The aim of this project is to develop and demonstrate a new capability for determining these signatures and inferring activities around critical assemblies. This will have a direct impact on the US government's nonproliferation, stockpile stewardship and nuclear forensics missions.

Technical Outcomes

This project successfully measured isotopic perturbations in uranium ores, demonstrating that they had experienced a natural neutron flux higher than that typically seen on earth. Irradiations were also carried out at the National Institute of Standards and Technology (NIST) Center for Neutron Research of concretes to attempt to generate similar isotopic perturbations under controlled conditions. This work was facilitated by improved analytical methods refined under this project.

Publications

Posters

Pollington, A. D., J. D. Inglis and S. M. K. Hanson. A new method for high-precision Sm isotope analyses: applications to natural and perturbed samples. Presented at *Goldschmidt Conference*, Barcelona, Spain, 2019-08-19 - 2019-08-19. (LA-UR-19-28231)

How Biological Communities Can Unlock Hidden Signatures of Environmental Change

Jeanne Fair
20180715PRD2

Project Description

The Science of Signatures (SOS) pillar links the Laboratory's capability to pressing national needs in the Laboratory's primary mission areas of National Security Science, Global Security, and Emerging National Challenges. It does so by developing a scientific understanding of the origin and evolution of signatures and backgrounds, new measurement techniques and strategies for signature identification, and new analysis and interpretation tools for development of knowledge from these signatures. This project seeks to identify signatures of biological communities from the microbiome to forest communities in response to environmental change. Application of biological community signatures is relevant to global health security and threat reduction with pathogen detection as well as environmental change over time.

Publications

Journal Articles

Abeyta, E. J., A. W. Bartlow, C. D. Hathcock and J. M. Fair. Individual nest site preferences do not explain upslope population shifts of a secondary cavity-nesting bird species. Submitted to *Proceedings of the Royal Society B. Biological Sciences*. (LA-UR-20-24957)

Ambrosiano, J. J., B. H. Sims, A. W. Bartlow, W. E. Rosenberger, M. R. Ressler and J. M. Fair. Ontology-Based Graphs of Research Communities: A Tool for Understanding Threat Reduction Networks. 2020. *Frontiers in Research Metrics and Analytics*. **5**. (LA-UR-19-31892 DOI: 10.3389/frma.2020.00003)

Bartlow, A. W., C. Machalaba, W. Karesh and J. M. Fair. Biodiversity and Global Health: Intersection of Health, Security and the Environment. Submitted to *Med One*. (LA-UR-19-32341)

*Bartlow, A. W., C. Manore, C. Xu, K. A. Kaufeld, S. D. Valle, A. Ziemann, G. Fairchild and J. M. Fair. Forecasting Zoonotic Infectious Disease Response to Climate Change: Mosquito Vectors and a Changing Environment. 2019. *Veterinary Sciences*. **6** (2): 40. (LA-UR-19-22170 DOI: 10.3390/vetsci6020040)

Bartlow, A. W., Z. R. Stromberg, C. D. Gleasner, B. Hu, K. W. Davenport, S. Jakhar, P. Li, M. Vosburg, M. Garimella, P. S. G. Chain, T. H. Erkkila, J. M. Fair and H. Mukundan. Quantifying Intrinsic Bias in Diagnosis of Human Upper Respiratory Tract Infections – Implications for Early Diagnosis of Emerging Threats. Submitted to *Frontiers in Microbiology*. (LA-UR-20-25518)

Bartlow, A. W. and S. Bush. Faunal turnover of rodents following pi\xc3\xb1on-juniper expansion in the Great Basin. Submitted to *Biodiversity and Conservation*. (LA-UR-20-22841)

Fair, J. M., J. Herman, C. D. Hathcock and A. W. Bartlow. A LONG-TERM STUDY OF THE EFFECTS OF BLOWFLIES ON THE GROWTH AND CONDITION OF SONGBIRD NESTLINGS. Submitted to *Oikos*. (LA-UR-20-24140)

*Musgrave, K., A. W. Bartlow and J. M. Fair. Long-term variation in environmental conditions influences host–parasite fitness. 2019. *Ecology and Evolution*. **9** (13): 7688-7703. (LA-UR-18-31593 DOI: 10.1002/ece3.5321)

Wysner, T. E., A. W. Bartlow, C. D. Hathcock and J. M. Fair. Long-term phenology of two North American secondary cavity-nesters in response to changing climate conditions. 2019. *The Science of Nature*. **106** (9-10): 54. (LA-UR-18-30750 DOI: 10.1007/s00114-019-1650-9)

Presentation Slides

Bartlow, A. W. How biological communities can unlock hidden signatures of environmental change. . (LA-UR-20-30013)

Bartlow, A. W. Biosurveillance of zoonotic diseases to promote global health security. . (LA-UR-21-22579)

Fair, J. M. Bird communities and climate change. Presented at *Bird communities and climate change*, Los Alamos, New Mexico, United States, 2018-11-06 - 2018-11-07. (LA-UR-18-30737)

*Jacobs, L., B. H. McMahon, J. Berendzen, J. Longmire, C. Gleasner, N. W. Hengartner, M. Vuyisich, J. R. Cohn, M. Jenkins, A. W. Bartlow and J. M. Fair. California condor microbiomes: Bacterial variety and functional properties in

captive-bred individuals. . (LA-UR-17-26676 DOI: 10.1371/journal.pone.0225858)

Improving Public Health by Linking Virus Genetic Evolution and Epidemic Spread

Arshan Nasir
20180751PRD3

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).

Publications

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. 2020. *Marine Genomics*. 100790. (LA-UR-20-23340 DOI: 10.1016/j.margen.2020.100790)

Mughal, F., F. Gul, A. Nasir and G. Caetano-Anolles. 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. From Ivanovski to Covid-19: Investigating the Concept and Origin of Viruses. Submitted to *Trends in Microbiology*. (LA-UR-20-24424)

Nasir, A., F. Mughal and G. Caetano-Anolles. The Tree of Life Describes a Tripartite Cellular World. Submitted to *Bioessays*. (LA-UR-20-30493)

*Nasir, A., G. Caetano-Anoll\xc3\xa9s 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)

*Romero-Severson, E., A. Nasir and T. K. 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)

An Atomtronic Rotation Sensor

Malcolm Boshier
20180753PRD3

Project Description

This research will develop one approach to creating a so-called waveguide Sagnac atom interferometer. This device acts as an exquisitely sensitive rotation sensor. Rotation sensors are a key component of inertial navigation systems (INS). The atom interferometer sensor could potentially improve positioning accuracy with INS by an order of magnitude. Such an advance would be viewed as extremely important by agencies within DOD and the Intelligence Community (IC) who need precise positioning when Global Positioning System (GPS) is unavailable or denied. The device may also function as an accelerometer or gravimeter, which can be useful for detecting underground facilities relevant to non-proliferation and for finding mineral and oil deposits relevant to fossil fuels.

Publications

Journal Articles

Kim, H., K. A. Krzyzanowska, C. Ryu, K. C. Henderson, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple-loop atom interferometer. Submitted to *arXiv.org*. (LA-UR-20-28166)

Presentation Slides

Kim, H. Waveguide atom interferometer at LANL. . (LA-UR-21-22793)

Posters

Kim, H., J. Ferreras Fuertes, K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu and M. G. Boshier. Progress Toward Atomtronics Sagnac Interferometer. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28645)

Kim, H., K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple round-trip waveguide atom interferometer. Presented at *APS DAMOP 2020*, Portland, Oregon, United States, 2020-06-01 - 2020-06-01. (LA-UR-20-23957)

Biophysical Interactions of Amphiphiles with Biomimetically Patterned Membranes

Loreen Stromberg
20190614PRD1

Project Description

Many of the biomarkers involved in infectious disease, cancer, and neurotraumatic conditions are lipids. The lipidic biochemistry is critical in determining the interaction of these biomarkers with membranes (which are also lipidic), blood, and other body fluids (which are aqueous). Yet, current methods for the measurement and detection of these biomarkers completely ignore their lipid biochemistry. Because of this, there is a significant failure rate in the adaptation of such technologies for real-world applications. Characterization, measurement, and understanding of these biomarkers in a physiological context can therefore revolutionize our ability to combat many conditions of relevance to human health. In this project, we will develop an ink-jet printing based method for the characterization and measurement of such lipidic biomarkers with membrane interactions, so as to enhance our understanding of human health without the need for animal models. This combines expertise in materials science, chemistry, modeling, and biological sciences and can provide new capabilities that can stretch beyond the biological sciences and influence materials science and environmental studies as well.

Publications

Presentation Slides

Stromberg, L. R. Interfacing Biomarkers and Materials Science: applications for detection and therapeutics. Presented at *Seminar for Chemical & Biological Signature Science Group at PNNL*, Richland, Washington, United States, 2021-01-13 - 2021-01-13. (LA-UR-21-20042)

Posters

Stromberg, L. R., J. H. Werner, G. A. Montano and H. Mukundan. LPS-induced bilayer deformation is modulated with increasing lipid membrane complexity. Presented at *2019 CINT User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29418)

Stromberg, L. R., J. H. Werner, G. A. Montano and H. Mukundan. LPS-Induced Bilayer Deformation is Modulated with Increasing Lipid Membrane Complexity. Presented at *Biophysical Society Meeting*, San Diego, California, United States, 2020-02-15 - 2020-02-19. (LA-UR-20-21298)

Disease Outcome Analysis for Improved Disease Interventions

Paul Fenimore
20190618PRD1

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.

Smart Mobile Sensor Platform Development for Radiological Mapping of Large-Scale Areas

Suzanne Nowicki
20190625PRD2

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.

Publications

Journal Articles

S. Shin, T. H., D. T. Wakeford and S. F. Nowicki. Multi-sensor optimal motion planning for radiological contamination surveys using prediction-difference maps. Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-20-26153)

Presentation Slides

S. Shin, T. H. Gaussian process regression for radiological contamination mapping. . (LA-UR-21-20338)

S. Shin, T. H. and S. F. Nowicki. Smart Mobile Sensor Platform Development for Radiological Mapping of Large-scale Areas. . (LA-UR-21-20339)

Development and Implementation of a Portable Microfluidic J-Coupled Spectrometer for Rapid Detection and Identification of Emerging Chemical Threats

Derrick Kaseman
20190641PRD3

Project Description

This project will invent and develop new approaches for the detection of chemical warfare agents, chemical threat agents, pesticides, and insecticides. The detector is designed as a portable system that can be implemented domestically and internationally to help combat terrorism. The overarching goal of this project is to optimize a portable, fieldable detector that only uses earth's very small magnetic field to detect and identify minute quantities of chemical threats. This will be accomplished by optimizing a microfluidics-based spectrometer with a new detection system that reduces, by 10-fold, the total volume of sample required and the amount of sample in the volume by 1000-fold. This project ties into other Department of Energy national security missions by developing a unique technique for signature based, portable chemical sensing, which has important applications for military defense and homeland security.

Publications

Journal Articles

*Kaseman, D. C., M. T. Janicke, R. K. Frankle, T. Nelson, G. Angles-Tamayo, R. J. Batrice, P. E. Magnelind, M. A. Espy and R. F. Williams. Chemical Analysis of Fluorobenzenes via Multinuclear Detection in the Strong Heteronuclear J-Coupling Regime. 2020. *Applied Sciences*. **10** (11): 3836. (LA-UR-19-30126 DOI: 10.3390/app10113836)

Kaseman, D. and S. Sen. A review of the application of 2D isotropic-anisotropic correlation NMR spectroscopy in structural studies of chalcogenide glasses. 2020. *Journal of Non-Crystalline Solids*. 120500. (LA-UR-20-26008 DOI: 10.1016/j.jnoncrysol.2020.120500)

Presentation Slides

Kaseman, D. Nuclear Magnetic Resonance of Complex Material Systems: From Glasses to Chemical Warfare Agents. . (LA-UR-19-31588)

Kaseman, D. Chemical Warfare Agents Detection via Portable Low-Field Nuclear Magnetic Resonance. Presented at *Techwatch*, Washington D.C., Virginia, United States, 2020-03-11 - 2020-03-11. (LA-UR-20-22174)

Kaseman, D. Chemical Analysis of Small Molecules via NMR at Earth's Magnetic Field. Presented at *ACS Fall 2020*, San Francisco, California, United States, 2020-08-17 - 2020-08-17. (LA-UR-20-25767)

Kaseman, D. Earth's Field NMR for Detection of Chemical Warfare Agents. . (LA-UR-20-28887)

Kaseman, D. New Frontiers in Earth's Field NMR for Structure Elucidation. Presented at *NMR**2*, Virtual, New Mexico, United States, 2020-11-13 - 2020-11-13. (LA-UR-20-28961)

Posters

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. New Frontiers in Nuclear Magnetic Resonance using Earth's Magnetic Field. . (LA-UR-19-28901)

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Identification of organophosphorus chemical warfare agents (CWAs), precursors, and decomposition products with a fieldable spectrometer using earth's magnetic field. Presented at *ACS Fall 2020*, San Francisco, California, United States, 2020-08-17 - 2020-08-17. (LA-UR-20-25766)

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Portable Earth's Field NMR Systems for the Detection of Chemical Warfare Agents. Presented at *PANIC*, La Jolla, California, United States, 2020-10-19 - 2020-10-22. (LA-UR-20-27477)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. A Fieldable Spectrometer Using Earth's Magnetic Field for Detection of Organophosphorus Nerve Agents. Presented at *Chemical and Biological Defense Science & Technology*, Cincinatti, Ohio, United States, 2019-11-17 - 2019-11-21. (LA-UR-19-31201)

Unraveling Lipoprotein Signatures for Tick-Borne Pathogens

Harshini Mukundan
20190655PRD4

Project Description

Vector borne pathogens present with different immunological signatures in the vector vs. the human host. These signatures are often the key towards unraveling their mode of action - be it immune evasion or activation- and lipidic molecules produced by the pathogen have a critical role to play in this response. In this project, we will use novel sensor technology together with lipoprotein measurement strategies in order to identify and unmask these critical signatures of Borrelia surface proteins, the causative agent of Lyme disease, in order to develop methods for rapid diagnostics and treatment of the infection.

The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting

Christopher Johnson
20200681PRD1

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

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)

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. Submitted to *Geophysical Research Letters*. (LA-UR-20-26366)

Xue, L., Y. Fu, C. W. Johnson, J. Otero-Tores, C. Shim and R. Burgmann. Seasonal seismicity in the Lake Biwa region of central Japan moderately modulated by lake water storage changes. Submitted to *Journal of Geophysical Research: Earth Surface*. (LA-UR-21-20003)

Presentation Slides

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)

The Next Generation of Aerosol Optical Models: Humidity Dependence and Chemical Processing

Manvendra Dubey
20200752PRD3

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

Sullivan, R. C., H. Boyer-Chelmo, K. J. Gorkowski and H. Beydoun. Using Aerosol Optical Tweezers to Explore the Evolution of Microdroplet Chemistry, Acidity, Phase Separations, and Morphology. Submitted to *Accounts of Chemical Research*. (LA-UR-20-24435)

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)

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)

Modeling an Artificial Radiation Belt of Ionized Fission Fragments After a High-altitude Nuclear Explosion (HANE)

Misa Cowee
20190528MFR

Project Description

The "Starfish mystery" refers to the unexpectedly widespread artificial radiation belt of beta-decay electrons created by the 1962 Starfish Prime High Altitude Nuclear Explosion (HANE) test shot, which fatally degraded ~1/3 of the satellites in orbit at the time. This widespread belt seemingly defied the laws of physics, as the ionized fission fragments which produced the beta-decay electrons should have been confined by magnetic fields, rather than transported far across them. A credible physical explanation of this effect has eluded the community for the last 50+ years, and is not included in current artificial radiation belt models. This lack of understanding is a limiting factor in our ability to accurately predict and prepare for this threat to satellites. In this project, we will develop a first-ever model to better understanding the motion and transport of ionized fission fragments on the seconds to hours timescales relevant to the formation of the belt taking into account several important loss processes. We will also better understand the threat posed to under-shielded satellites components, such as solar panels, from the ionized fission fragments themselves. Such knowledge is important to DOE/NNSA for predicting the man-made space environment and satellite hardening standards.

Publications

Journal Articles

Engel, M. A., M. Cowee, V. K. Jordanova, G. S. Cunningham, Y. Chen and D. Larson. Simulation of the Formation and Evolution of an Artificial Belt of Ionized Fission Fragments. Submitted to *Journal of Radiation Effects Research and Engineering*. (LA-UR-20-23666)

Books/Chapters

Jordanova, V. K. CHAPTER 6: Ring Current Decay. (LA-UR-19-32034)

Reports

Chen, Y., M. A. Engel, V. K. Jordanova, M. Cowee, G. S. Cunningham and D. J. Larson. On the Radiation Effects of Strontium Ions on Satellite Solar Cells in Low Earth Orbits. Unpublished report. (LA-UR-21-20757)

Presentation Slides

Cowee, M. Artificial Radiation Belt Phenomenology Modeling. . (LA-CP-20-20502)

Cowee, M. Artificial Radiation Belts: Phenomenology and Modeling. . (LA-UR-20-27458)

Cowee, M. Artificial Radiation Belt Modeling at LANL. . (LA-UR-20-27529)

Cowee, M., V. K. Jordanova, M. A. Engel, Y. Chen and G. S. Cunningham. LANL LDRD Mission Foundations Project Update: Modeling an Artificial Radiation Belt of Ionized Fission Fragments After a HANE. . (LA-UR-20-30064)

Engel, M. A., M. Cowee, V. K. Jordanova, Y. Chen and G. S. Cunningham. Simulation of the Formation and Evolution of an Artificial Belt of Ionized Fission Fragments. Presented at *HEART*, Liousiville, Kentucky, United States, 2020-03-23 - 2020-03-27. (LA-UR-20-22361)

Posters

Engel, M. A., M. Cowee, V. K. Jordanova, S. K. Morley and M. G. Henderson. Impact of Loss Processes on Modeling the Ring Current. Presented at *American Geophysical Union Fall Meeting 2019*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32277)

How Can the Granular Defects of Additive Manufacturing be Evaluated?

Carly Donahue
20200495MFR

Project Description

Additive Manufacturing (AM) is currently revolutionizing fabrication of metal parts and is of growing importance in global security and weapons applications. This project will use novel techniques to analyze additively manufactured parts for defects. Department of Defense (DOD) and Department of Energy (DOE) weapons programs benefit from this work by allowing the parts to be non-destructively tested and verified to be of the required integrity before entering service. There are currently programs within the DOE weapons complex to do analysis of parts and determine what defects are problematic to material and part properties. Since inspection is an important part of technology and part qualification National Institute of Standards and Technology (NIST) is also working closely in these areas. National Aeronautics Space Administration (NASA) and the Federal Aviation Administration (FAA) are currently working on projects to accelerate adoption of AM-produced parts for aerospace applications. This research will have a significant impact on the ability to qualify a part for service in all industries. These defects are difficult if not impossible to detect through conventional non-destructive techniques making the proposed method very valuable.

Publications

Other

Donahue, C. M. and C. J. Montgomery. Acoustic Data of Additively Manufactured Parts as part of LDRD MFR. Dataset. (LA-UR-20-23833)

Non-Destructive Analysis and Surveillance of Containers used for Nuclear Material Storage

Rajendra Vaidya
20190505MFR

Project Description

Nuclear material storage and handling is a critical component to the plutonium manufacturing and non-proliferation missions at Los Alamos National Laboratory, and there are more than 5000 containers of stored nuclear materials at Technical Area 55 at Los Alamos. The projected increase in the programmatic scope over the next few years is expected to highlight the need for improved and efficient material storage and accountability. There is a strong and immediate need to develop non-destructive inspection techniques for nuclear material storage containers which can monitor internal damage and corrosion processes in-situ. The current destructive tests used on these containers are time consuming, expensive, and are also performed on a relatively small subset of the current population. Non-destructive testing can be used to significantly increase the fraction of storage containers inspected and can provide real time results in a short amount of time. If successful, the proposed testing methodologies will increase the current sampling from 10's of containers/year to 100's/year, and it will reduce the costs of destructive testing by a factor of 3 (minimum based on conservative estimates). This could save the Federal Government almost $2.5 M a year while ensuring 100% testing.

Technical Outcomes

The Modular Non-destructive Test System (MINTS) team successfully integrated three Non-destructive Evaluation (NDE) techniques into one single platform. The combination of the three NDE techniques viz. ultrasonic testing, eddy current testing, and laser interferometry will allow the team to interrogate corrosion effects in nuclear material storage containers. The Gantry system coupled with the positioning and rotational capabilities will allow the testing of different sizes of containers in a short period of time.

Publications

Journal Articles

Vaidya, R. U., M. N. Davenport, A. A. Abeyta and A. S. Guider. Non-Destructive Analysis of SAVY Containers: Application of Non-Destructive Testing to Assess Corrosion Damage. Submitted to *Journal of Nuclear Materials Management*. (LA-UR-18-21194)

Conference Papers

Vaidya, R. U., J. G. Gigax, A. A. Abeyta and M. N. Davenport. Application of Non-Destructive Testing to Assess Corrosion Damage in Nuclear Material Storage Containers. Presented at *PATRAM (Packaging and Transportation of Nuclear Materials)*. (New Orleans, Louisiana, United States, 2019-08-04 - 2019-08-09). (LA-UR-19-23273)

Vaidya, R. U., J. G. Gigax, A. A. Abeyta and M. N. Davenport. Recent Updates on the Application of Non-Destructive Testing to Assess Corrosion Damage in SAVY Containers. Presented at *International Nuclear Materials Management 60th Annual Meeting*. (Palm Desert, California, United States, 2019-07-14 - 2019-07-18). (LA-UR-19-23536)

Presentation Slides

Vaidya, R. U., J. G. Gigax, A. A. Abeyta and M. N. Davenport. Recent Updates on the Application of Non-Destructive Testing to Assess Corrosion Damage in SAVY Containers. Presented at *60th Annual International Nuclear Materials Management Conference*, Palm Desert, California, United States, 2019-07-14 - 2019-07-18. (LA-UR-19-26022)

Predictive Science for Inverse Problems in Non-proliferation

Thomas Burr
20200456MFR

Project Description

Department of Energy, National Nuclear Security Administration, and Department of Homeland Security tackle inverse problems that involve measured gamma and/or neutron counts. The project application uses gamma spectra to infer which radioisotopes are present and in what amounts in test items. Although forward modelling is currently used, this project will improve the relevant forward model while allowing for model bias in the context of solving the inverse problem. Then, once a forward model is validated for use in the inverse problem, the model can become an explicit component of the inverse approach. A forward model that is validated for the inverse provides a means to perform predictive science for the inverse problem, by solving the inverse problem on simulated data. Currently, performance claims regarding how well the inverse can be solved are typically optimistic on simulated data. For example, the actual percentage of correctly inferring which isotopes are present could be 70% while the predicted percentage might be 90% or more. This project aims for more credible forward modelling, explicit use of the improved forward model in the inverse approach, and aims to provide a strategy to confirm how well performance on the inverse can be predicted.

Technical Outcomes

Using previously-collected gamma spectra used a subset of 300 available gamma spectra to refine the data generator, implemented and evaluated a new radio-isotope identification option based on approximate Bayesian computation (ABC) that uses the refined data generator, and assessed performance on measured spectra and improved synthetic spectra This project made an adaptation needed to ABC to “calibrate” the data generator to allow for model bias while experimenting with summary statistics such as net peak areas.

Publications

Journal Articles

Burr, T. L., S. Croft, A. Favalli, T. Krieger and B. P. Weaver. Bottom-up and Top-Down Uncertainty Quantification for Measurements. Submitted to *Chemometrics and Intelligent Laboratory Systems*. (LA-UR-20-27332)

Secure, Robust Multimedia Wireless Sensor Networks for Monitoring Critical Energy Infrastructure

David Mascarenas
20200506MFR

Project Description

The Los Alamos Engineering Institute has developed a technique known as VideoMagic to automatically extract resonant frequencies, vibrational mode shapes and damping ratios from video of vibrating structures. This technique estimates full-field mode shapes at high spatial resolution. The ability to capture full-field mode shapes at high spatial resolution allows quantitative analysis of mode shapes for detecting small losses of stiffness in structures. VideoMagic's most sensitive characterization of damage to-date is detecting/ locating a 3% loss in stiffness in an aluminum beam. This performance is an order-of-magnitude better than the nearest competing contact-sensor based technique. Because this technique is based on video measurements it has very low installation costs in comparison to competitors. This project developed techniques to make VideoMagic robust against motion of the imager and the structure undergoing monitoring. Preliminary results suggest the technique is robust against atmospheric scintillation when used to analyze video of structure captures over a non-trivial distance. This technology has great potential for difficult renewable-energy monitoring challenges such as monitoring the state-of-health of an off-shore wind turbine farm, infrastructure associated with fossil fuel extraction (e.g. offshore oil rigs, riser cables), and electricity generation facilities.

Technical Outcomes

This project extended the Blind-Source Separation – based video structural identification algorithm to accommodate traveling waves. The team began the development of tools for simulating photorealistic video of vibrating structures in order to aid in planning the deployment of imager sensor networks for monitoring critical infrastructure such as wind turbines. Finally, the team developed a privacy-preservation/steganography extension to the video-based structural dynamics algorithms for enhanced security.

Publications

Presentation Slides

L. Mascarenas, D. D., A. W. Green, M. F. Silva and B. Martinez. Sparse and Random Sampling Techniques for High Resolution, Full Field, BSS Based Structural Dynamics Identification from Video. Presented at *ISR -2 Seminar Series*, Los Alamos, New Mexico, United States, 2020-12-17 - 2020-12-17. (LA-UR-20-30255)

L. Mascarenas, D. D., A. W. Green, M. F. Silva and B. Martinez. Privacy Preserving Structural Dynamics. Presented at *International Modal Analysis Conference*, Online, New Mexico, United States, 2021-02-08 - 2021-02-08. (LA-UR-20-30473)

Silva, M., A. W. Green, E. Figueiredo, J. Costa and D. D. L. Mascarenas. A Generalized Technique for Full-field Blind Identification of Travelling Waves and Complex Modes from Video Measurements with Hilbert Transform. Presented at *International Modal Analysis Conference*, online, New Mexico, United States, 2021-02-08 - 2021-02-08. (LA-UR-21-20025)

Other

L. Mascarenas, D. D. Multi-Camera Video-Based Sensor Networks for Digital Twin Generation: From the city-scale to micron-scale. Audio/Visual. (LA-UR-20-22822)

L. Mascarenas, D. D. Video-Based Structural Dynamics for Automated Model Generation and Updating. Audio/Visual. (LA-UR-20-27088)

L. Mascarenas, D. D., A. W. Green, J. E. Morales Garcia, A. Cattaneo and M. Anghel. Summer 2020 Imager Dynamics Dataset. Dataset. (LA-UR-20-26006)

L. Mascarenas, D. D., A. W. Green and J. E. Morales Garcia. Thin Vibrating Structure Video Dataset. Dataset. (LA-UR-20-25080)

L. Mascarenas, D. D. and A. W. Green. Imager Data 8/10/2020. Dataset. (LA-UR-20-26406)

L. Mascarenas, D. D. and A. W. Green. 8_21_2020_Imager_Dataset. Dataset. (LA-UR-20-26640)

L. Mascarenas, D. D. and J. E. Morales Garcia. Multi-Time of Flight Imager Dataset. Dataset. (LA-UR-20-20329)

Meyerhofer, P. D. and D. D. L. Mascarenas. Ultrasound simulations for the microreactor. Audio/Visual. (LA-UR-20-26001)

Advanced Signatures, Processing, and Exploitation for Counter-proliferation (ASPEC)

Kevin Mitchell
20190651DI

Project Description

Remote sensing provides great operational value to the nonproliferation mission. Sensors must be regularly calibrated to ensure that their sensitivity is understood as they age. Existing calibration targets have limitations in their ability to support sensitivity calibration because of environmental uncertainties in the calibration scene. This project implements a new methodology for calibration target fabrication that removes the environmental uncertainties to create a new paradigm for sensor calibration. Additionally, existing analysis tools require significant subject matter expertise to use, and still do not effectively exploit all the information that is available. This project will explore the limits of the possible in remote sensing data analysis, and will develop analysis tools that can be used by non-specialists.

Publications

Reports

Duque, J. G., N. G. Parra-Vasquez, G. L. Wagner, L. R. Stromberg, H. Mukundan, J. J. Crochet and K. L. Mitchell. BETELGEUSE:Spectral Exploration of Biological Signatures for Remote Sensing Applications An LDRD-Director’s Initiative. Unpublished report. (LA-CP-20-20299)

Presentation Slides

Duque, J. G., N. G. Parra-Vasquez, G. L. Wagner, J. J. Crochet and K. L. Mitchell. Detection and Identification of Biological Materials with Remote Sensing Techniques. . (LA-CP-20-20796)

Emerging Challenges in Space and Earth Science

Lisa Danielson
20180475CR

Project Description

This project provides national science research & education services that benefit a wide range of Los Alamos National Laboratory's national security programs in global security, energy and climate security and space situational awareness, and the modeling capability in the stockpile stewardship program. This includes university research outreach and student / postdoc research programs, which are the technical heart of this project. This project further provides funding for new ideas and programs that may play a large part in the future DOE/ NNSA mission. Support for innovative small work also plays a large role in the Lab's retention of technical talent.

Publications

Journal Articles

*Abeysekara, A. U., A. Albert, R. Alfaro, C. Alvarez, R. Arceo, J. C. Arteaga-Velazquez, D. A. Rojas, H. A. A. Solares, E. Belmont-Moreno, S. Y. BenZvi, C. Brisbois, K. S. Caballero-Mora, A. Carraminana, S. Casanova, J. Cotzomi, S. C. de Leon, C. De Leon, E. De la Fuente, S. Dichiara, B. L. Dingus, M. A. DuVernois, J. C. Diaz-Velez, K. Engel, C. Espinoza, H. Fleischhack, N. Fraija, A. Galvan-Gamez, J. A. Garcia-Gonzalez, M. M. Gonzalez, J. A. Goodman, J. P. Harding, B. Hona, F. Hueyotl-Zahuantitla, P. Huntemeyer, A. Iriarte, A. Lara, W. H. Lee, H. L. Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, J. Lundeen, K. Malone, S. S. Marinelli, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, J. A. Matthews, P. Miranda-Romagnoli, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, M. U. Nisa, R. Noriega-Papaqui, E. G. Perez-Perez, Z. Ren, C. D. Rho, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, H. Salazar, F. S. Greus, A. Sandoval, M. Schneider, G. Sinnis, A. J. Smith, R. W. Springer, K. Tollefson, I. Torres, G. Vianello, T. Weisgarber, J. Wood, T. Yapici, A. Zepeda, H. Zhou and J. D. Alvarez. Searching for dark matter sub-structure with HAWC. 2019. *Journal of Cosmology and Astroparticle Physics*. **2019** (07): 022. (LA-UR-18-31168 DOI: 10.1088/1475-7516/2019/07/022)

*Banerjee, T., T. Holland, K. Solander, M. Holmes and R. Linn. Identifying Characteristics of Wildfire Towers and Troughs. 2020. *Atmosphere*. **11** (8): 796. (LA-UR-19-30049 DOI: 10.3390/atmos11080796)

*Bonneville, A., R. Kouzes, J. Yamaoka, A. Lintereur, J. Flygare, G. S. Varner, I. Mostafanezhad, E. Guardincerri, C. Rowe and R. Mellors. Borehole muography of subsurface reservoirs. 2018. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*. **377** (2137): 20180060. (LA-UR-18-26169 DOI: 10.1098/rsta.2018.0060)

*Bonneville, A., R. T. Kouzes, J. Yamaoka, C. Rowe, E. Guardincerri, J. M. Durham, C. L. Morris, D. C. Poulson, K. Plaud-Ramos, D. J. Morley, J. D. Bacon, J. Bynes, J. Cercillieux, C. Ketter, K. Le, I. Mostafanezhad, G. Varner, J. Flygare and A. T. Lintereur. A novel muon detector for borehole density tomography. 2017. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **851**: 108-117. (LA-UR-16-27062 DOI: 10.1016/j.nima.2017.01.023)

S. Boyce, S. H., Z. Lei, B. J. Euser, E. E. Knight, E. Rougier, J. Stormont and M. Reda-Taha. Simulation of mixed-mode fracture using the combined finite–discrete element method. 2020. *Computational Particle Mechanics*. **7** (5): 1047-1055. (LA-UR-19-32443 DOI: 10.1007/s40571-020-00341-6)

Caldwell, W. K., A. Hunter, C. S. Plesko and S. Wirkus. Understanding Asteroid 16 Psyche’s composition through 3D impact crater modeling. 2020. *Icarus*. **351**: 113962. (LA-UR-19-32428 DOI: 10.1016/j.icarus.2020.113962)

Chen, G., H. Fu, Y. Zhang, X. Li, Y. Ge, A. Du, C. Liu and Y. Xu. Energetic Electron Acceleration in Unconfined Reconnection Jets. Submitted to *Astrophysical Journal Letters*. (LA-UR-19-28967)

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Cote, B., M. Eichler, A. Yague, N. Vassh, M. R. Mumpower, B. Vilagos, B. Soos, A. Arcones, T. M. Sprouse, R. Surman, M. Pignatari, B. Wehmeyer, T. Rauscher and M. Lugaro. Constraining the rapid neutron-capture process with meteoritic 129-I and 247-Cm. Submitted to *Science*. (LA-UR-19-30942)

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Posters

N. Albright, M. B., L. A. Gallegos-Graves, J. C. Thompson, R. Johansen, D. Ulrich, K. L. Avery, B. Timalsina, K. K. Stringfield, A. C. Runde, D. L. Lopez, T. M. Yoshida, M. Shakya, S. A. Sevanto and J. M. Dunbar. Principles for Microbiome Engineering. . (LA-UR-19-28938)

Bloser, P. F., W. T. Vestrand, L. P. Parker, D. C. Poulson, M. I. Pinilla-Orjuela, K. Smith, A. S. Hoover, S. F. Nowicki, A. V. Klimenko and R. M. Kippen. Experimental Gamma-Ray Astronomy at Los Alamos National Laboratory. Presented at *The 36th Annual New Mexico Symposium*, Online, New Mexico, United States, 2020-11-13 - 2020-11-13. (LA-UR-20-29262)

Caldwell, W. K., A. Hunter, C. S. Plesko and S. Wirkus. Impact Crater Models of Asteroids in Forthcoming NASA Missions. Presented at *Lunar and Planetary Science Conference*, The Woodlands, Texas, United States, 2020-03-16 - 2020-03-20. (LA-UR-20-22013)

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Froment, M. Seismic Modeling of Meteorite Impacts on the Surface of Mars.. . (LA-UR-20-25070)

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Guardincerri, E., C. A. Rowe, E. S. Schultz-Fellenz, C. Morris, J. D. Bacon, J. M. Durham, D. J. Morley, K. O. Plaud-Ramos, D. C. Poulson, M. Roy, N. George, A. Bonneville and R. Kouzes. 3D Tomography of a Mesa Using Cosmic Ray Muons Detected in an Underground Tunnel. Presented at *AGU Fall Meeting*, San Francisco, California, United States, 2016-12-12 - 2016-12-16. (LA-UR-16-29293)

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Other

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Miller, J. M., J. Lippuner, R. T. Wollaeger, T. M. Sprouse and M. R. Mumpower. Simulations of Neutrino-Driven Accretion Flows. Dataset. (LA-UR-20-29317)

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