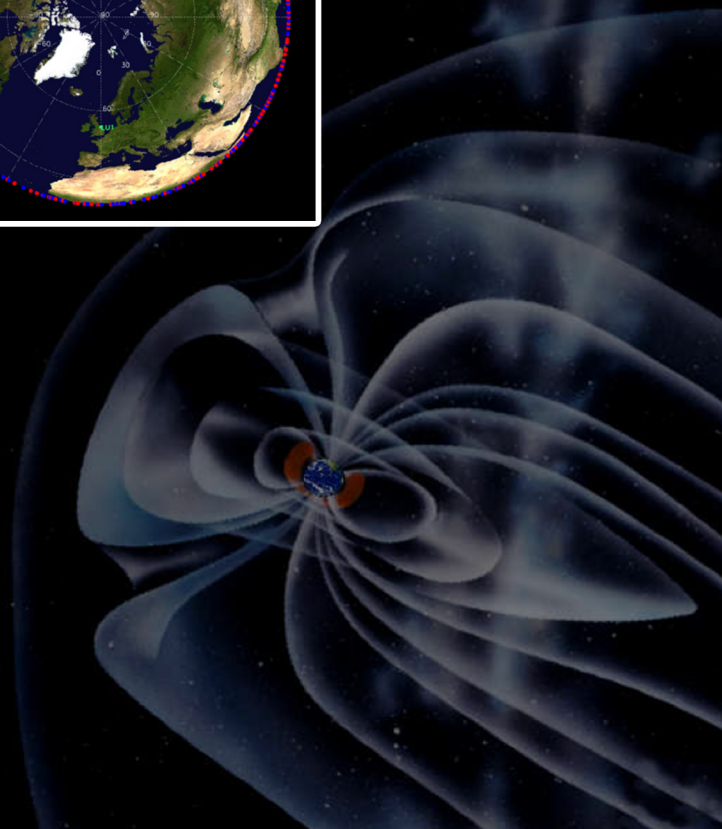
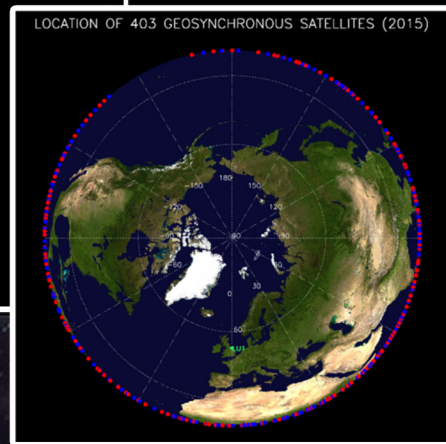
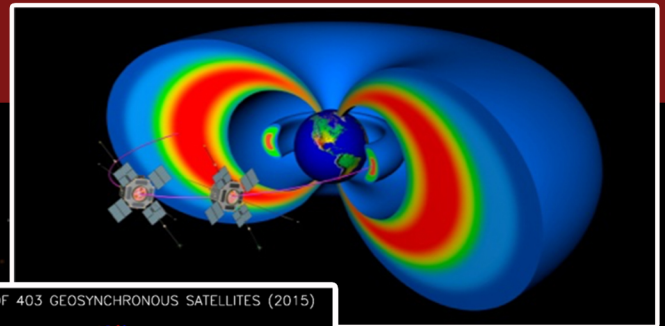



FY17 ANNUAL PROGRESS REPORT

Laboratory Directed Research and Development

Los Alamos National Laboratory



About the Cover

Space Hazards Induced near Earth by Large, Dynamic Storms (SHIELDS) is a tool for modeling the complex near-Earth environment for space assets protection and space situational awareness. SHIELDS protects communication, navigation and scientific satellites orbiting Earth's magnetosphere by predicting hazards resulting from solar storms that cause space weather. Space weather could damage onboard electronics in satellites and thus interrupt radio and television reception, disrupt the operation of cellphones and GPS, shut down the Internet and endanger military and civilian operations. Researchers developed the software platform to understand, model and predict this weather about an hour before it hits satellites, enabling instruments to be placed in a safe mode. SHIELDS is the winner of a 2017 R&D 100 Award, submitted by Los Alamos National Laboratory with the University of Michigan. Vania Jordanova led the Los Alamos team of Gian Luca Delzanno, Humberto Godinez, J. David Moulton, Daniil Svyatsky, Michael Henderson, Steve Morley, Jesse Woodroffe, Thiago Brito, Christopher Jeffery, Alin-Daniel Panaitescu, Collin Meierbachtol, Earl Lawrence and Louis Vernon. University of Michigan collaborators included Gabor Toth, Daniel Welling, Yuxi Chen and John Haiducek. The LDRD program invested in SHIELDS through Directed Research projects 20140061DR and 20150033DR. 



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Structure of this Report

In accordance with U.S. Department of Energy Order (DOE) 413.2C, the Laboratory Directed Research and Development (LDRD) annual report for fiscal year 2017 (FY17) provides summaries of each LDRD-funded project for the fiscal year, as well as full final reports on completed projects. The report is organized as follows:

Overview: An introduction to the LDRD program at Los Alamos National Laboratory (LANL), the program's structure and strategic values, the LDRD portfolio management process, and highlights of outstanding accomplishments by LDRD researchers.

Project Summaries: The project summaries are organized by Focus Areas – 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 FY17.

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.

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Overview

Laboratory Directed Research and Development is a prestigious source of research and development funding at the Los Alamos National Laboratory. It follows a strategic guidance derived from the missions of the U.S. Department of Energy, the National Nuclear Security Administration, and the Laboratory. To execute that strategy, the Los Alamos LDRD program creates a free market for ideas that draws upon the bottom-up creativity of the Laboratory's best and brightest researchers. The combination of strategic guidance and free-market competition provides a continual stream of capabilities that position the Laboratory to accomplish its missions.

The LDRD program provides the Laboratory Director with the opportunity to strategically invest in forward-thinking, potentially high-payoff research that strengthens the Laboratory's capabilities to address national security challenges. Funded in FY17 with approximately 5.5% of the Laboratory's overall budget, the LDRD program helps the Los Alamos anticipate, innovate, and deliver world-class science and engineering.

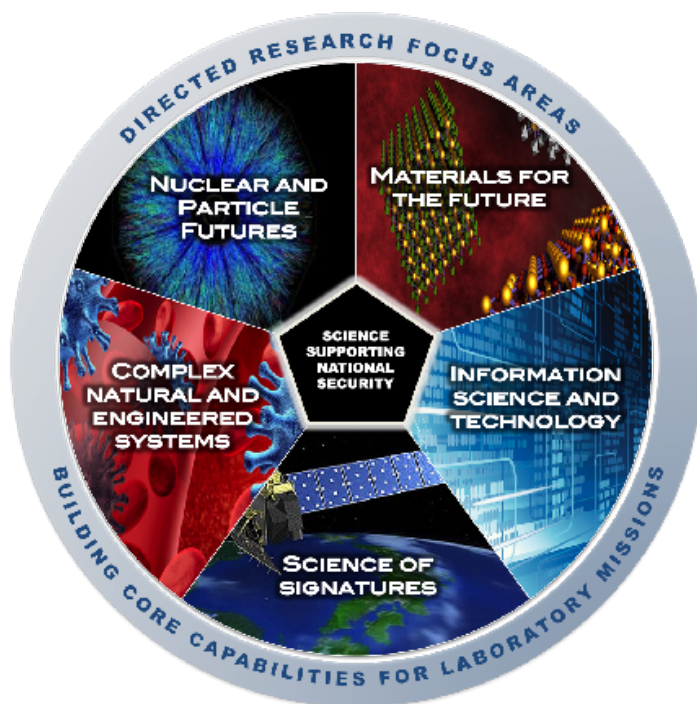
Program Structure

The Los Alamos LDRD program is organized into five program components with distinct institutional objectives: Directed Research (DR), flagship investments in mission solutions; Exploratory Research (ER), smaller projects that invest in people and skills that underpin key Laboratory capabilities; Early Career Research (ECR), supporting the development of early-career researchers; Mission Foundations Research (MFR), translating discovery into innovative solutions; and Postdoctoral Research and Development (PRD), recruiting bright, qualified, early-career scientists and engineers. In FY17, the LDRD program funded 298 projects with total costs of \$118 million. These projects were selected through a rigorous and highly competitive peer review process and are reviewed formally and informally throughout the fiscal year. The LDRD Program Office holds a reserve each year to make modest investments that address new opportunities. In FY17, the reserve budget was approximately \$3.5M.

Directed Research

The DR component makes long-range investments in multidisciplinary scientific projects in key competency or technology-development areas. In FY17, LDRD funded 45 DR projects, which represents approximately 53% of the program's research funds. Directed Research projects are typically funded up to a maximum of \$1.7M per year for three years.

Directed Research is organized around Focus Areas that define key areas of science, technology, and engineering in support of Los Alamos missions. The Focus Areas map to the Los Alamos science pillars, plus an additional multi-disciplinary Focus Area that is not captured by the pillars. Between them, they capture the capabilities that are essential to our Laboratory missions in the long term (3-15 years). For each Focus Area, coordinators led a process to engage broadly with the Lab to set investment priorities for the FY17 Strategic Investment Plan, published labwide.



Exploratory Research

The ER component is focused on developing and maintaining technical staff competencies in key strategic disciplines that form the foundation of the Laboratory's readiness for future national missions. Largely focused on a single discipline, ER projects explore highly innovative ideas that underpin Laboratory programs. In FY17, LDRD funded 144 ER projects, which represents approximately 35% of the program's research funds. Exploratory Research projects are funded up to an average maximum of \$350K per year for three years.

Unlike DR proposals, division endorsements are not required for ER proposals; instead, this component of the LDRD program is operated as an open and competitive path for every staff member to pursue funding for his/her great idea. The ER component is a critical channel for purely bottom-up creativity at the Laboratory. Nonetheless, it is strongly driven by mission needs via the definition of the 12 ER research categories, and the assignment of investment between them.

Directed Research Focus Areas	Mission Impact
Information Science and Technology	Advance theory, algorithms, and high-performance computing to accelerate the integrative and predictive capability of the scientific method.
Materials for the Future	Rapidly meet mission needs based on a thorough knowledge of materials properties and interactions in relation to composition, structure, and scale.
Science of Signatures	Apply science and technology tools to extremely complex problems in signature, identification, and characterization, understanding, control or mitigation.
Nuclear and Particle Futures	Advance fundamental and applied nuclear science, including accelerator science and technology, in support of all Laboratory missions.
Complex Natural and Engineered Systems	Understand, predict, integrate, design, engineer, and/or control complex systems that significantly impact national security, particularly those involving energy, infrastructure, or societal sustainability.

Exploratory Research Technical Categories	Capability Development
Biological, Biochemical, and Cognitive Sciences	Biosciences
Chemistry and Chemical Sciences	Chemistry
Computational and Numerical Methods	Information and knowledge sciences, computer and computational sciences
Computer Science, Mathematics, and Data Science	High-performance computing, data analysis, and data-driven science
Defects and Interfaces in Materials	Theoretical, computation and modeling, and experimental methods to understand defects and interfaces in materials
Earth and Environmental Sciences and Space Physics	Earth and space sciences
Engineering Applications	Weapons science and engineering, advanced manufacturing, sensors, and remote sensing
Emergent Phenomena in Materials Functionality	Theory, computation and modelling, and experimental methods to understand behavior of materials
High-energy Density, Plasma, and Fluid Physics	High-energy density plasmas and fluids and beams
Measurement Science, Instrumentation, and Diagnostics	Measurement methods that enable new scientific discovery
Nuclear and Particle Physics, Astrophysics, and Cosmology	Nuclear physics, astrophysics, and cosmology
Quantum and Optical Science	Fundamental interactions and excitations in atomic, optical, and molecular systems

Early Career Research

The ECR component of the LDRD program is designed to strengthen the Laboratory’s scientific workforce by providing support to exceptional staff members during their crucial early career years. The intent is to aid in the sometimes challenging transition from postdoc to full-time staff member, and to stimulate research in disciplines supported by the LDRD program. In FY17, the LDRD program funded 25 ECR projects, which represents approximately 4% of the program’s research funds. Early Career Research projects are funded up to \$225K per year for two years, and only up to 60% of the project leader’s overall funding can be from the LDRD program.

Postdoc Research and Development

The PRD component ensures the vitality of the Laboratory by recruiting outstanding researchers. Through this investment, the LDRD program funds postdoctoral fellows to work under the mentorship of PIs on high-quality projects. The primary criterion for selection of LDRD-supported postdocs is the raw scientific and technical talent of the candidate, with his or her specialty a secondary factor. In FY17, LDRD funded 75 PRD projects, which represents 7% of the program’s research funds. These postdocs are supported full-time for two years.

In addition to approximately 57 Director’s Postdocs, the LDRD program supported 15 distinguished postdoctoral fellows at a higher salary and for a three-year term. Distinguished postdoctoral fellow candidates typically show evidence of solving a major problem or providing a new approach or insight to a major problem and show evidence of having a major impact in their research field. To recognize their role as future science and technology leaders, these appointments are named after some of the greatest leaders of the Laboratory’s past.

More postdocs are hired through DR and ER projects than directly through PRD appointments. Counting both avenues, in FY17 the LDRD program supported 53% of the 497 postdocs who spent at least part of the year at the Laboratory. The average population throughout the year was 263.

Mission Foundations Research

Initiated in FY17, the underlying objective of Mission Foundations Research (MFR) is to translate discovery into innovative solutions. The MFR component funds applied science and engineering in the technology readiness level (TRL) 3-5 range, targeting mission problems defined in advance by mission champions across the Laboratory. Technical readiness levels are used by many federal agencies, such as the U.S. Department of Homeland Security, to estimate the maturity of a technology. Proposed MFR projects must be at TRL 2 and have a solid scientific foundation. In FY17, the LDRD program funded nine MFR projects, which represents \$1.7 million total investment.

FY17 MFR Projects	
Title	Problem Statement
Pellet Cracking During Fabrication of Pu-238 Oxide Fuel	Manufacturing Process Agility and Innovation
Ignis: A Cognitive RF Sensing LPDI Modem	Dominance of the Electromagnetic Spectrum
Direct Electrolytic Reduction of Plutonium Oxide Surrogates	Manufacturing Process Agility and Innovation
Active Microwave Beam Steering Using a Metasurface Approach	Dominance of the Electromagnetic Spectrum
Enhanced X-Ray Computed Tomography for Plutonium Manufacturing	Manufacturing Process Agility and Innovation
Additive Manufacturing of Hierarchical Multi-Phase High-Entropy Alloys for Nuclear Components	Exploiting Additive Manufacturing for Fabricating Radiation-tolerant Nuclear Components
Coherent Radio Frequency Collection Through Computation for CubeSat Constellations	Dominance of the Electromagnetic Spectrum
Insensitive High Explosives using PATO	Alternative Insensitive High Explosive
Laser Additive Manufacturing of P92 Steel for Radiation Tolerant Nuclear Components	Exploiting Additive Manufacturing for Fabricating Radiation-Tolerant Nuclear Components

■ Project selected for Phase II funding in FY18

Selecting and Managing LDRD Projects

The LDRD program is the vehicle by which the Laboratory harvests the ideas of some of our best and brightest scientists and engineers to execute DOE/NNSA missions. This bottom-up approach is balanced by a program management strategy in which Senior Laboratory leadership sets science and technology priorities, then opens an LDRD competition for ideas across the breadth of the Laboratory. Panels formed from the Laboratory's intellectual leaders rigorously review proposals. Conflict of interest is carefully regulated, and evaluation criteria include innovation and creativity, potential scientific impact, viability of the research approach, qualifications of the team and leadership, and potential impact on Laboratory missions. The selection processes are modeled on best practices established by the National Science Foundation (NSF) and National Institutes of Health (NIH).

To guarantee fairness and transparency, and to ensure that the strongest proposals are funded, the selection panels include managers and technical staff drawn from the full range of technical divisions. Serving on an LDRD selection panel is often a starting point on the path to leadership roles in the scientific community. Past LDRD panelists have gone on to be Laboratory Fellows, division leaders, program directors, association Fellows, and chief scientists, while others have become leaders in academia.

Benefits of Serving on LDRD Panels

The mission of the Laboratory is to solve the nation's most difficult national security problems. By their nature, these problems lack a well-defined path to solution. In fact, the path is often completely unknown. It is rare that such creative work is done alone; the ideas and results from many colleagues are needed, often drawn out in conferences, hallway conversations, journals, and seminars. LDRD is an internal arena in which Laboratory staff serve as peer reviewers and play a key role of interaction in the scientific process. Proposal selection panelists are chosen for their subject-matter expertise, and the discussions in which they engage are not only critical to the LDRD process, but they also provide an opportunity for panelists to educate themselves on the latest results and practices, and expose themselves to opportunities for collaboration. As noted in an evaluation of peer review conducted by the UK House of Commons, "Peer review is regarded as an integral part of a researcher's professional activity; it helps them become part of the research community."

Annual Project Appraisals

In FY17, the LDRD Program Office reviewed every multi-year project funded in the previous year. This occurred in various formats, from formal appraisals with external reviewers, to assessments organized by line managers, to informal visits with PIs, to written appraisals of ended projects. The primary objective of the reviews is to assess progress and provide peer input to help PIs maintain the highest quality of work. They also help the LDRD Program Office manage the program portfolio.

Continuing DR projects are appraised in their second and third years, with external reviewers playing an important role in the review that takes place in the second year. The internal-external review is open to all Laboratory staff. Four project appraisers – two internal and two external – are nominated by the PI and approved by the LDRD Program Director. When appropriate, the appraisal is held as part of a broader workshop hosted by the Laboratory. The Chair of the project appraisal panel is responsible for writing a formal report of the review that details how well a project is addressing and meeting its goals, and documents any weaknesses the panel may have observed. The PI is then required to respond to the concerns documented in the report with a revised project plan. The average score for second-year DR projects appraised in FY17 was 4.0, or "excellent."

Written reviews, held in the LDRD archives, address: (1) Brief summary of accomplishments; (2) Assessment of quality of science and technology, relevance to Laboratory and national missions, progress toward goals and milestones, project leadership, and the degree to which the project may establish or sustain a position of scientific leadership for the Laboratory; and (3) Recommendations by the committee for changes in the scope or approach of the project. The criteria for the most important point – number (2) above – are derived from criteria developed by the National Academy of Science to assess all federally sponsored research.

In addition to formal project appraisals, which are conducted annually, the LDRD Program Director and Deputy Program Director meet informally with PIs in their labs to discuss their projects. The purpose of these one-on-one meetings is to give PIs individualized assistance and to determine what the LDRD Program Office can do to positively impact the success of the project.

Continuing ER and ECR projects are appraised in their first and second years. The LDRD Deputy Program Director collaborates with the technical divisions to conduct project appraisals. Like DRs, the projects are appraised according to the federal criteria of quality, performance, leadership, and relevance.

Mission Relevance

Mission relevance is one of the most important criteria in the evaluation of a potential LDRD project; it is carefully considered in project selection and tracked annually through the data sheet process. Many of the technologies that put Los Alamos on the map have deep roots in LDRD and are valuable to DOE/NNSA mission areas of nuclear security, energy security, environmental remediation, and scientific discovery and innovation. LDRD work also benefits the national security missions of the Department of Homeland Security, the Department of Defense, and Other Federal Agencies. As a result, the scientific advances and technology innovations from LDRD provide multiple benefits to all Los Alamos stakeholders, consistent with Congressional intent and the Laboratory’s scientific strategy.

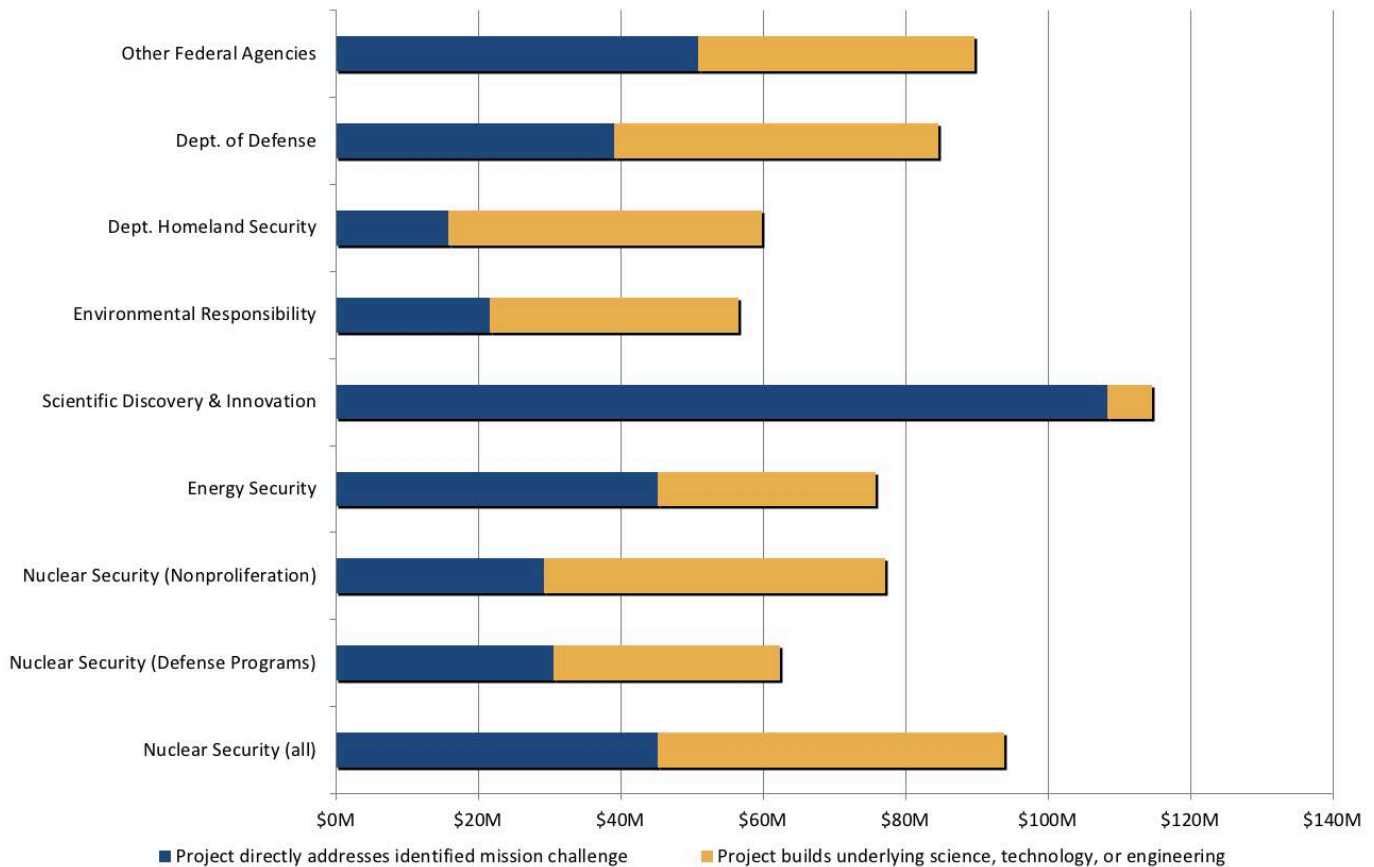
Los Alamos Science Goes Big in 2017

With a top-story list populated by breakthroughs in super-computing, accelerator science, space missions, materials science, life science, and more, Los Alamos put its science capabilities to wide, productive use in 2017.

“Teamwork across the disciplines from biology and biotech to astrophysics and space science drives our innovation in support of the Laboratory’s national security mission,” says Alan Bishop, Principal Associate Director for Science, Technology and Engineering at Los Alamos.

Many of the Laboratory’s significant achievements in FY17 were made possible by past or current LDRD investments in either the direct technology that was developed, or in the underlying capabilities that enabled it.

Mission Impact of FY17 LDRD Portfolio (\$M)



First and foremost, Los Alamos LDRD projects are required to address one or more of the DOE/NNSA mission areas. Due to the nature of basic R&D, the work may also benefit the mission challenges of other federal agencies. The multi-mission impact of LDRD projects is captured in the chart above, which is why the total expected benefit is approximately double the actual costs of the program in FY17.

TOP STORIES

2017

“No discipline left untouched—that’s the story from Los Alamos in 2017. In a remarkably productive year, Laboratory researchers grabbed headlines for their research in everything from physics to explosives modeling to HIV vaccine developments. ”

Alan Bishop, Principal Associate Director for Science, Technology and Engineering

Here’s a look at just a few of the Laboratory’s top science stories from 2017, with links to videos or articles about the work. All of the discoveries, advancements, or technologies mentioned here have roots in LDRD—some resulted from investments made as far back as 20 years ago, while others reflect recent LDRD investments in new capabilities that enable the Laboratory’s agile response to emerging national security challenges.



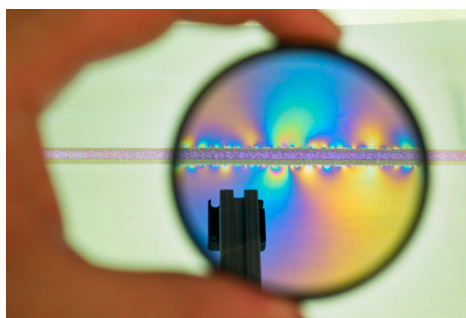
Trinity Supercomputer lands on two top-10 lists

It made number three on the High Performance Conjugate Gradients (HPCG) Benchmark project and number seven on the Top500 list. Working with the National Nuclear Security Administration, the Laboratory applies the capabilities of Trinity to providing assessments that ensure the nation’s nuclear stockpile is safe, effective and secure. The LDRD program funded a special call for Trinity science proposals in FY15 as part of the Laboratory’s system stabilization activities. The Laboratory made large parts of the Trinity system available to a select group of users for open science. [YouTube](#)



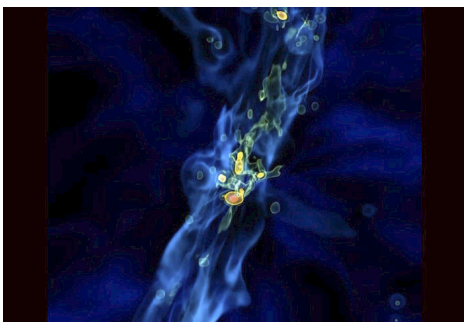
Rover findings indicate stratified lake on ancient Mars

Boron was discovered in calcium-sulfate veins on Mars using the ChemCam instrument on NASA’s Curiosity rover. Boron compounds play a role in stabilizing sugars needed to make RNA, a key to life. Los Alamos National Laboratory developed the laser-shooting Chemistry and Camera (ChemCam) instrument that sits atop Curiosity in collaboration with the French space agency. ChemCam applies the Laser Induced Breakdown Spectroscopy capability that was developed at Los Alamos with support from the LDRD program. [READ MORE](#) ↗



Machine-learning earthquake prediction in lab shows promise

By listening to the acoustic signal emitted by a laboratory-created earthquake, a computer science approach using machine learning can predict the time remaining before the fault fails. Los Alamos researchers developed a 2D tabletop simulator that models the buildup and release of stress along an artificial fault. At any given instant, the noise coming from the lab fault zone provides quantitative information on when the fault will slip. This work, supported by the LDRD program, has potential significance to earthquake forecasting, as well as nondestructive testing of many other failure scenarios. [READ MORE](#) ↗



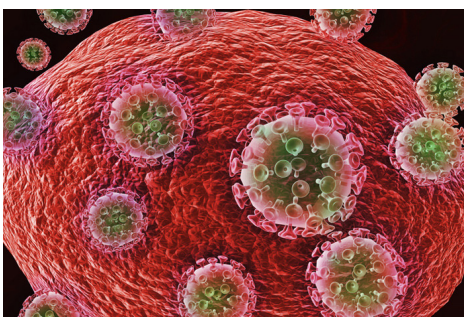
Breaking the supermassive black hole speed limit

Using computer codes for modeling the interaction of matter and radiation related to the Lab's stockpile stewardship mission, scientists simulated collapsing stars that resulted in supermassive black holes forming in less time than expected, cosmologically speaking—in the first billion years of the universe. A key mission area at Los Alamos National Laboratory is understanding how radiation interacts with certain materials. Because supermassive black holes produce huge quantities of hot radiation, their behavior helps test computer codes designed to model the coupling of radiation and matter. [YouTube](#)



Quantum dots amplify light with electrical pumping

Los Alamos–designed quantum dots achieve a breakthrough with electrical stimulation, showing the feasibility of a new generation of highly flexible, electrically pumped lasers processable from solutions that can complement or even eventually displace existing laser diodes. These prospective devices can enable a variety of applications, from RGB laser modules for displays and projectors to multi-wavelength micro-lasers for biological and chemical diagnostics. The work on the quantum dot synthesis and device fabrication was supported by the LDRD program. [READ MORE](#) >



Los Alamos research fundamental to the first efficacy study for mosaic HIV-1 preventative vaccine

International partners announced the first efficacy study for an investigational HIV-1-preventive “mosaic” vaccine. Janssen Pharmaceutical Companies of Johnson & Johnson are joining forces with The Bill & Melinda Gates Foundation and NIH on the study. The HIV-1 mosaic vaccine in the trial was originally designed at Los Alamos by theoretical biologist Bette Korber and her team. She was initially funded by LDRD to develop the concept and over the years has continued the work under various collaborative NIH grants. [READ MORE](#) >



Eight Los Alamos innovations win R&D 100 Awards

Since 1978 Los Alamos has won more than 145 of the prestigious R&D 100 Awards, and in 2017 it took eight, plus an innovation award. “The R&D 100 Awards represent the breadth, depth and innovation of the science and engineering at our Laboratory. They also reflect our partnerships with other government laboratories, universities and private industry,” said former Los Alamos National Laboratory Director Charlie McMillan. Four of the 2017 awards have roots in LDRD and represent the program's investments in science, engineering, and technology impacting the broader scientific community. [READ MORE](#) >

Performance Metrics

The impacts of the LDRD program are particularly evident in the number of publications and citations resulting from LDRD-funded research, the number of postdoctoral candidates supported and converted by the program, and the number of awards bestowed on scientists and engineers supported by the program. The following performance metrics reflect data available as of the publication of this report.

Publications

The LDRD program produces a large volume of high-quality scientific contributions relative to its portion of the Laboratory's budget. The numerous publications made possible with LDRD funding help the Laboratory maintain a strong presence and scientific reputation in the broader scientific community. In FY17, LDRD researchers generated 586 peer-reviewed publications, accounting for 26% of the Laboratory's total peer-reviewed publications. The quality of these publications is evidenced by the number of times they were cited. LDRD publications published in FY17 were cited 1,925 times, accounting for 32% of the Laboratory's citations.

Intellectual Property

Another indication of the cutting-edge nature of research funded by LDRD is the contribution the program makes to the Laboratory's intellectual property. As of the publication of this report, metrics of intellectual property generated at the Laboratory in FY17 are not available. Looking back five years, from FY13 to FY16, the LDRD program supported 25% of the Laboratory's patents granted and 32% of its invention disclosures. Given that LDRD continues to select research projects for their scientific excellence, it can be anticipated that metrics for FY17 will continue this trend of strong contribution to the Laboratory's intellectual property.

Postdoc Support

In an increasingly competitive job market, LDRD remains an important vehicle for recruiting the brightest researchers to Los Alamos National Laboratory, where they become innovators and scientific leaders. In FY17, LDRD supported 263 postdocs, accounting for 53% of the Laboratory's total. LDRD is also instrumental in retaining new talent from the postdoc pool at the Laboratory; of the 69 postdocs who converted to staff in FY17, 54% were supported by LDRD.

Postdoctoral Distinguished Performance Awards

The Laboratory established the Postdoctoral Distinguished Performance Awards to honor outstanding postdoc achievements that significantly impact the Laboratory's scientific efforts and status in the scientific community. The awards also recognize outstanding creativity, innovation, or level of performance substantially beyond what is expected of a Laboratory contributor at the postdoc level. All 2017 winners were supported by the LDRD program.



Maryline Ferrier is a current Postdoctoral Research Associate. The Award recognizes her outstanding research and leadership in actinide chemistry, specifically her investigation of the chelation chemistry of actinium. Worldwide interest in actinium-225 as a potential radiopharmaceutical anti-cancer agent motivated her

research. She conducted the first in a series of unique actinium coordination chemistry studies, which resulted in two papers in **Nature Communication** and **ACS Central Science**. Ferrier used extended x-ray absorption fine structure (EXAFS) experiments to make the first measurement of the length of an actinium bond. She overcame significant hurdles to work with extremely radioactive materials and led efforts to analyze her experimental results by combining x-ray absorption fine structure (XAFS) and multidimensional discrete Fourier transform (MDDFT). It is not often that a researcher can examine the macroscopic coordination chemistry of an element for the first time. Ferrier's accomplishments greatly extend the Lab's pioneering methods for realistic synthetic and characterization studies of radioactive elements.



Alex Zylstra is a former Reines Distinguished Postdoc Fellow and current Lab scientist. The Award honors him for his outstanding research and leadership in developing a new inertial confinement fusion (ICF) platform with the potential to revolutionize the field. The flagship of the US Inertial Confinement Fusion program, National Ignition Facility (NIF), seeks to achieve a self-sustained fusion nuclear reaction in the deuterium-tritium (DT) fuel by compressing the DT ice with high power lasers. This path requires a high convergence ratio, giving rise to instabilities and preventing the fuel from igniting. Zylstra has led the experimental part of the alternative approach, which utilizes the liquid DT fuel instead. This leads to smaller required convergence ratios, greatly improving the performance of the laser driven fuel implosions.

The campaign led by Zylstra gave the results, which would be considered an extreme success even for a senior scientist. He demonstrated the future prospects of the new concept with only three shots at NIF. The journal **Physical Review Letters** highlighted the resulting publication as an “Editor’s Suggestion”.

Zylstra currently leads an LDRD Early Career Research project that aims to measure the energy loss of charged particles in dense plasmas at various conditions to distinguish between theoretical models. The project will conduct novel experiments at the OMEGA and NIF laser facilities to obtain essential data in this parameter space of critical importance to fusion and other high-energy-density plasmas. The data will be used to validate or exclude various theoretical models of the stopping power. Refined models can then be incorporated into hydrodynamics simulations of high-energy-density plasmas, such as ignition experiments on the NIF where charged-particle stopping of the fusion-produced alpha particles provides the plasma self-heating. This work has potential to impact the Laboratory’s stockpile stewardship mission.



Thomas Myers is a former Director’s Postdoc Fellow and current Lab scientist. The Honorable Mention Award recognized him for his outstanding research and leadership in the general field of energetic materials, in particular for the design and synthesis of photoactive energetic materials. The latter work has the potential to make a profound impact in the field of detonator design, where materials that have significant stability with respect to mechanical, thermal, and electrostatic insult can be selectively initiated using an infrared laser pulse. The Journal of the American Chemical Society published this research.

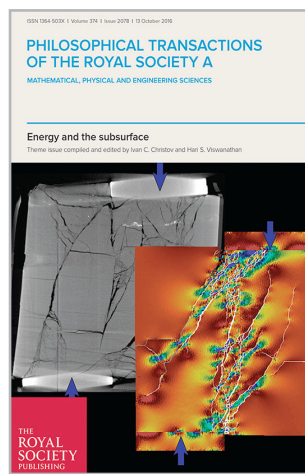
During Myers’s tenure as a postdoc, he synthesized more than 50 new energetic materials, published or submitted ten manuscripts in top-tier journals describing these new materials, and gave three invited talks and submitted one patent application. In addition, he developed and received approval for a new safety test at LANL, which enables the rapid and efficient screening of these photoactive materials by using samples that are less than 50 mg. Myers also supported the instrumentation needs of his group and coworkers. His work has attracted considerable interest, funding, and collaborations from the defense community.

On the Cover and Beyond

- The numerous publications made possible with LDRD funding help Los Alamos maintain a strong presence and scientific reputation in the broader scientific community. Not only does the program support a significant fraction of the Laboratory's publications, it also supports much of the research featured on the covers of peer-reviewed journals. These are just a few examples from FY17.

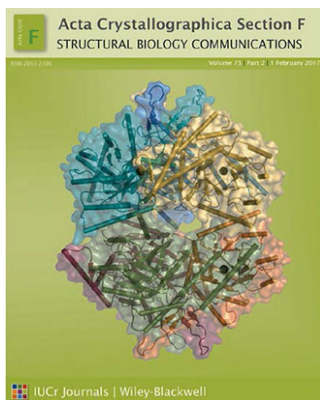
Understanding the multi-scale problem of hydraulic fracturing

Hydraulic fracturing (also known as fracking) has had a substantial impact on the energy sector by providing access to hydrocarbons in low permeability formations that were previously inaccessible. However, the physical mechanisms that control its efficiency and environmental impacts remain poorly understood in part because the relevant length scales range from nanometers to kilometers. Hari Viswanathan has led a team performing an integrated experimental and computational assessment of the key phenomena in hydraulic fracturing that control the production of hydrocarbons. **Philosophical Transactions of the Royal Society A** published the work in the "Energy and the Subsurface" theme issue and featured it on the journal's cover. Ivan Christov (Purdue University, formerly at LANL) and Viswanathan co-edited the issue. The theme for the journal issue arose from an international Geological Fluid Mechanics Conference sponsored by the Lab's Center for Nonlinear Science and Center for Space and Earth Science (CSES). Issue contributors were selected from attendees of the Conference. National Academy of Science members, a National Academy of Engineering member, former CNLS director Robert Ecke, editors from leading technical journals, and prominent oil and gas industry scientists also contributed to the issue.



The LDRD program and DOE Fossil Energy-National Energy Technology Laboratory Unconventional Oil and Gas funded different aspects of the work.

X-ray crystal protein structure helps elucidate function



Acetyl-coenzyme A (acetyl-CoA) is a key component of metabolism. It contributes an acetyl group to the Krebs cycle so that it can be oxidized for energy production in a cell. Lab researchers seek to understand the generation of acetyl-CoA for energy applications. The team used the Stanford Synchrotron Radiation Light Source to examine the structure of the malyl-coenzyme A lyase (malyl-CoA lyase) enzyme, which catalyzes a reaction to create acetyl-CoA and glyoxylate. These enzymes are found in a variety of bacteria, where they are involved in the assimilation of one- and two carbon compounds. **Acta Crystallographica** published their findings of the structure and understanding of how the structure contributes to the enzyme's function. The journal featured the x-ray crystal structure of malyl-CoA lyase on its cover. With this new understanding of the mechanism of the malyl-CoA enzyme, the team has begun experimenting with its use as a carbon-neutral way to produce acetyl-CoA. Normally, an acetyl-CoA-producing reaction releases carbon dioxide (CO₂). However, the reaction uses the malyl-CoA enzyme to produce a 2-carbon molecule,

glyoxylate, which can be further metabolized to other products. This pathway could potentially improve lipid biosynthesis in micro-algae, a biofuel feedstock.

The LDRD program funded the work.

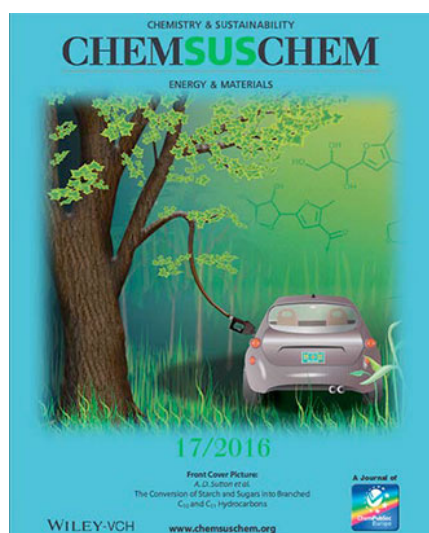
First synthesis and characterization of the actinium aquo ion

Actinium-225 is a particularly promising isotope for targeted anticancer therapy because it emits alpha particles that are suitable for therapeutic use, and it decays to the biologically innocuous bismuth-209 isotope. However, scientific and technical challenges remain in understanding the coordination chemistry that will allow effective biological delivery of this promising isotope. A Los Alamos team has been studying various fundamental aspects of actinium chemistry with the intent of realizing its medical potential. Developing an understanding of the actinium ion in water is critical for characterizing chemical equilibria that define metal complexation in biologically relevant systems. The journal **ACS Central Science** published their research and featured it on the cover.

The LDRD program and Office of Basic Energy Sciences funded different aspects of the work. Los Alamos Institutional computing provided computational resources through the Wolf Cluster. The DOE Isotope Development and Production for Research and Application subprogram within Office of Nuclear Physics supplied the Actinium-225.



Converting sugars into hydrocarbon fuels



A Los Alamos team is investigating methods to convert biomass into fuels. Sources of fossil-based hydrocarbons, such as heavy oil, shale gas, and oil sands, have helped address the decline of global fossil fuels production. Because these are finite resources, sustainable and renewable alternatives to petroleum are needed to fill future gaps in the supply of transportation fuels and chemical feedstocks. Renewable, non-food-based biomass is considered to be one of the most promising alternatives for the production of fuels and commodity chemicals. The Lab researchers are developing a mild route starting from simple sugars to prepare branched alkanes suitable for diesel fuel. **Chemistry & Sustainability** (ChemSusChem) published the research and featured it on the journal cover.

The Lab team has succeeded in converting sugars into linear alkanes containing between 8 and 16 carbon atoms through selective aldol chain extension of 5-hydroxymethylfurfural (5-HMF) followed by ring-opening and hydrodeoxygenation. This process allowed them to isolate hydrocarbons in up to 95 % yield. The use of bio-derived furans, such as 5-HMF, has also been exploited by others to produce alkanes, and cellulose has been used directly to make pentane and

hexane. The team has eliminated some processing steps and is moving towards “raw biomass” as the primary process input, rather than commodity chemicals produced from biomass.

The project began with support from the LDRD program, and the DOE Office of Energy Efficiency & Renewable Energy (EERE) Bioenergy Technology Office later funded the concept.

Awards and Recognitions

The LDRD program helps Los Alamos National Laboratory anticipate, innovate, and deliver solutions to some of the nation's toughest challenges. The driving force behind each impact has been the focused initiative of many talented scientists and engineers who choose to apply their knowledge and expertise in service to the nation. The LDRD program is proud to support the work of some of the Laboratory's most accomplished researchers, who in FY17 received many prestigious awards, honors, and recognitions.



International Union of Pure and Applied Chemistry Award

The International Union of Pure and Applied Chemistry (IUPAC) selected Jaqueline L. Kiplinger as one of 12 women to be honored with a 2017 Distinguished Women in Chemistry or Chemical Engineering Award. She is the first Los Alamos scientist to receive this recognition. The IUPAC Award honors Kiplinger for her groundbreaking work in establishing synthetic routes to novel uranium and thorium compounds that have opened new frontiers in understanding the nature of bonding and reactivity in actinides. She currently leads an LDRD project focused on preparing and studying a new class of actinide compounds, which is expected to open new frontiers in synthesis, spectroscopy, molecular and electronic structures of actinide materials.

In 2017, Kiplinger was also selected by the Iota Sigma Pi (the National Honor Society of Women in Chemistry) to receive the 2017 Violet Diller Professional Excellence Award. The award is given triennially to recognize contributions to chemistry that have had widespread significance to the scientific community or society on a national level. The award honors her scientific achievements, service to the broad chemistry community and mentoring of early career researchers. She presented a summary of her work and received the award during a ceremony at the July 2017 Iota Sigma Pi national convention.



Fellow of the American Chemical Society

The American Chemical Society (ACS) has selected James M. Boncella (Inorganic, Isotope and Actinide Chemistry, C-IIAC) as a 2017 Fellow. The Fellows Program recognizes members who have made exceptional scientific contributions and who have provided excellent volunteer service to the ACS community. Boncella joins just five other Laboratory scientists with the rank of ACS Fellow.

The ACS chose Boncella for his seminal discoveries in actinide chemistry and his long and distinguished history of service to the ACS, including serving as Chair of the Division of Inorganic Chemistry. His current LDRD project aims to generate fundamental chemical understanding necessary to enable the fabrication of a chemical gas generation system that could replace large, heavy gas pressure bottles for performing pressure-based work.



Fellow of the American Physical Society

Han Htoon was cited for “pioneering accomplishments in development of single nanostructure, optical spectroscopy/imaging techniques, elucidating fundamental/quantum optical processes of quantum dots and single wall carbon nanotubes, and device integration of optical nanomaterials.

Htoon’s current LDRD project aims to establish covalently doped nanotubes as a new path toward realizing quantum information technologies.



Laura Beth Smilowitz was cited for “pioneering radiography to study thermal explosions, including the development of both a scaled tabletop dynamic radiographic facility capable of producing continuous X-ray movies of high-speed events and the triggering techniques required to observe the spontaneous onset of a thermal explosion.”

Smilowitz lends her technical expertise as a reviewer on LDRD peer-review panels charged with reviewing and selecting proposals for funding according to their mission relevance and scientific merit.



Vivien Zapf was cited for “seminal contributions to the understanding of quantum mechanical properties of superconductors, quantum magnets and multiferroic systems at low temperatures and in extreme magnetic fields to 100T.”

In her current LDRD project, Zapf is performing measurements of bulk antiferromagnetic properties, X-ray light source characterization of antiferromagnetic domains and theoretical modeling to understand the origin of antiferromagnetic domains. She also serves on peer-review panels to select Exploratory Research projects.



Fellow of The Optical Society

The board of directors of The Optical Society (OSA) elected Hou-Tong Chen as an OSA Fellow. The OSA cited Chen for “seminal contributions to the field of metamaterials, including active metamaterials and the realization of novel electromagnetic structures at terahertz frequencies.”

Chen leads an LDRD project that will develop a novel device architecture for quantum dot light emission devices, based on opportunities arising from metamaterials and epsilon-near-zero materials, affording superior performance compared to the current state-of-the-art.



Complex Natural and Engineered Systems

Physiological and Structural Acclimation to Climate Change in Forest Ecosystems

Sanna Sevanto
20160670PRD3

Project Description

The proposed work is to conduct studies of the plasticity and acclimation of forest trees in response to experimental reductions in precipitation and elevations in temperature. Multi-factor experiments are rare but invaluable for studying the response of trees to climate change. Furthermore, research on acclimation to climate change has often been conducted on tree seedlings in controlled growth chambers with few studies in natural settings. This project will use a Los Alamos field experiment where whole-tree chambers and rain exclusion systems have been established to control both soil moisture and atmospheric temperature for two tree species presenting contrasting physiological responses to drought. The knowledge of tree acclimation acquired through this project will provide valuable information for the calibration and validation of climate-vegetation models.

Publications

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- Grossiord, C., S. Sevanto, T. E. Dawson, H. D. Adams, A. D. Collins, L. T. Dickman, B. D. Newman, E. A. Stockton, and N. G. McDowell. Warming combined with more extreme precipitation regimes modifies water sources of trees. 2017. *New Phytologist*. **213**: 584-596. <http://onlinelibrary.wiley.com/doi/10.1111/nph.14192/abstract>.
- Grossiord, C., S. Sevanto, I. Borrego, A. M. Chan, A. D. Collins, L. T. Dickman, P. J. Hudson, N. McBranch, S. T. Michaletz, W. T. Pockman, M. Ryan, A. Vilagrosa, and N. G. McDowell. Tree water dynamics in a drying and warming world. . 2017. *Plant, Cell & Environment*. **40**: 1861-1873.

Development and Application of Multi-scale Models for Disease Forecasting

Carrie Manore
20160662PRD2

Project Description

We will examine three specific examples of infectious disease outbreaks as case studies to develop science-based decision support, including model development, uncertainty quantification, and risk communication. As a result of this work, we will have a greater understanding of the lessons to be learned from three specific epidemics of enormous importance to global public health: the West African Ebola outbreak of 2014, the emergence of virulence and antibiotic resistance in high disease-burden environments, and the spread of vector-borne disease. From these studies, we will also gain insights into how demographics, climate change, and policy decisions can influence these and other cases of disease emergence. This work addresses the Laboratory's global security mission.

from field transmission experiments. 2017. *Letters in Biomathematics*. **3** (1): 209-228.

Xue, , C. A. Manore, Thongsripong, and J. M. Hyman. Two-sex mosquito model for the persistence of Wolbachia. 2017. *JOURNAL OF BIOLOGICAL DYNAMICS*. **11** (1): 216-237.

Publications

Manore, C. A., M. I. Teboh-Ewungkem, O. Prosper, A. L. Peace, K. Gurski, and Z. Feng. Intermittent preventive treatment (IPT): Its role in averting disease-induced mortalities in children and in promoting the spread of antimalarial drug resistance. 2017. *arXiv preprint*. <http://https://arxiv.org/abs/1701.05210>.

Shutt, D., C. A. Manore, S. Pankavich, A. Porter, and S. Y. Del Valle. Determining important Zika outbreak characteristics via approximate Bayesian computation for epidemics in South and Central America. To appear in *Epidemics*.

Manore, C. A., R. S. Ostfeld, F. B. Agosto, Gaff, and S. L. LaDeau. Defining the Risk of Zika and Chikungunya Virus Transmission in Human Population Centers of the Eastern United States. 2017. *PLOS NEGLECTED TROPICAL DISEASES*. **11** (1).

Hilker, F. M., L. J. S. Allen, V. A. Bokil, C. J. Briggs, Feng, K. A. Garrett, L. J. Gross, F. M. Hamelin, M. J. Jeger, C. A. Manore, A. G. Power, M. G. Redinbaugh, M. A. Rua, and N. J. Cunniffe. Modeling Virus Coinfection to Inform Management of Maize Lethal Necrosis in Kenya. 2017. *PHYTOPATHOLOGY*. **107** (10): 1095-1108.

Kaplan, M., C. A. Manore, and K. H. Bagamian. Agent-based hantavirus transmission model incorporating host behavior and viral shedding heterogeneities derived

Evolution of Water and CO₂ at Mars: Implications for its Past and Future

Katherine Mesick
20160672PRD3

Project Description

Non-polar regions on Mars with near surface water deposits indicated by Mars Odyssey neutron data will be studied. Our work will provide key information in understanding the context for forming these equatorial water deposits on Mars, and what Mars' past climate was like. These answers will provide vital information on the history of water on Mars and the potential for future human exploration. This work also supports the nuclear nonproliferation mission area with space-based instruments capable of detecting nuclear explosions in the atmosphere and space.

Impacts of Climate and Land Use on Global River Dynamics

Joel Rowland
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.

Investigations of the Magnetic Characteristics of Iron-Only Clusters

John Gordon
20160255ER

Project Description

This project will develop new iron clusters as these molecules have the potential to behave as single-molecule magnets. The expected high magnetic spins of these clusters may lend themselves to applications such as quantum computing and high-density information storage using spintronics. The use of spintronics technologies could potentially revolutionize the electronics and computing industries by making it possible to store vastly more data in devices than is currently possible. Efficient spintronics technologies could mean huge energy savings due to the fact that reversing the electronic spins in such systems would require less power than the normal electronic charge. This work will build capabilities in theory, computation and modeling, and experimental chemistry that form the foundation for understating new synthetic materials.

Forecasting Failure

Paul Johnson
20170673PRD2

Project Description

A large earthquake in Cascadia or California would devastate the regional and potentially national economies. The primary national security challenge the 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 anthropogenic ally induced seismicity, particularly in the mid west. 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.

Publications

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Advanced Technology Laser Triggering of High Power Linear Induction Accelerator Pulsed Power Switches

Roger Shurter
20170625ER

Project Description

This project will lead to the development of high energy, multi-kilojoule pulsed power switches with highly precise temporal resolution. With the application of these new switch designs using pressured air rather than the asphyxiants currently in use such as sulfur hexafluoride, the Science Based Stockpile Stewardship program may be significantly impacted. A potential example of this technology application is the new down-hole radiographic research accelerator under development for sub-critical weapons testing at the Nevada Test Site.

Design of New Materials for Energy Applications

Ping Yang
20170684PRD3

Project Description

The scientific results of this project will not only spark further experimental verification of the proposed redox flow cells, but will also be used as a general guideline towards the realization of novel inexpensive, safe, and high-performance flow cells, which could be implemented in electricity grids in the near future. This project directly responds to the aim of approaching DOE's cost target on large-scale energy storage, \$150/kWh. Having developed such systems, people will be able to effectively store and use greener electricity rather than relying on carbon energy sources, such as fossil fuels, which the world will run out of sooner or later.

Tandem Dehydrogenation of Formic Acid and Olefin Hydrogenation: Steps Towards a Self-Sustaining Pressure/Volume System

James Boncella
20170685PRD3

Project Description

The goal of this project is to generate the fundamental chemical understanding necessary to enable the fabrication of a chemical gas generation system that will replace large, heavy gas pressure bottles for performing pressure-based work. This will be accomplished through the generation of a tandem catalysis system that will perform two functions. It will decompose formic acid to hydrogen and carbon dioxide, and also use some of the hydrogen that is produced in the reaction to perform a separate reaction that will generate the heat necessary to drive the decomposition of formic acid at a practical rate. Such a reaction system would be an enormous advance to catalytic science because it would necessitate a detailed understanding of how to accomplish multi-step chemical transformations in a single reaction vessel.

Publications

Anderson, N. H., J. M. Boncella, and A. M. Tondreau. Reactivity of Silanes with ((PONOP)-P-tBu)Ruthenium Dichloride: Facile Synthesis of Chloro-Silyl Ruthenium Compounds and Formic Acid Decomposition. 2017. *CHEMISTRY-A EUROPEAN JOURNAL*. **23** (55): 13617-13622.

Regulation of Intercellular Signaling

Angel Garcia
20160676PRD4

Project Description

G-protein coupling receptors (GPCR) are a large family of proteins that detect external signals (e.g., light or molecules) on a cell's surface and trigger a cell response. Cell responses can range from opening a channel that leads to a nerve system signal, or to trigger cell division. GPCRs are the target of over 50% of approved drugs in the market. However, the mechanisms of action of GPCRs are not known at the molecular level. Understanding the mechanism of action can help understand diseases at the molecular level, which in turn can help design new drugs. This project employs high performance computational tools to simulate the dynamics of GPCRs in environments that mimic the cell surface. The simulations are validated with experimental data available in the literature. A comparison of atomistic simulation data with in cell data enables the postulation and testing of hypotheses about the mechanism of action of these proteins.

Publications

Systems biology at LANL: integration of experiment, theory and computation. 2017. *PADSTE funded workshop and report on LANL capabilities in systems biology.*

Neale, C., R. Pomès, R. Sterne-Marr, and A. García. Protein Folding upon Binding Revealed by Molecular Dynamics Simulation. 2017. *Biophysical Journal (abstract)*. **112** (3): 54a. [http://www.cell.com/biophysj/abstract/S0006-3495\(16\)31359-5](http://www.cell.com/biophysj/abstract/S0006-3495(16)31359-5).

Ye, L., C. Neale, A. Sljoka, A. E. García, O. P. Ernst, and R. S. Prosser. Mechanistic insights into allosteric regulation of the A2A Adenosine G-protein-coupled receptor by physiological cations. To appear in *Nature Communications*.

Neale, C., and R. Pomès. Sampling errors in free energy simulations of small molecules in lipid bilayers. 2016. *Biosimulations of lipid membranes coupled to experiments*. **1858** (10): 2539-2548. <http://www.sciencedirect.com/science/article/pii/S0005273616300839>.

Expediting the Genetic Engineering of Microalgae for Industrial Production

Scott Hennelly
20160393ER

Project Description

This work in algal research will drive its development as an industrially viable systemic technology. Using genetic tools we will elucidate the algal genome and make algal genetic engineering more routine. Extensive genetic manipulations are required to realize algae's inherent potential as a systemic technology. To date, progress has been slow, due to poorly characterized algal genetics and a lack of genetic tools such as plasmids, reliable transformation methods and viral vectors. Our goal is to make algal genetic engineering routine. We will deliver a set of tools and methods to deliver genes to algae, stably integrate them into the genome, and express them. Beyond simple feedstock for energy production, harnessing the complex biosynthetic power algae would open new avenues for the production of a wide array of complex chemicals and materials of interest for national security applications.

Molecular Actinide Nitrides

Marisa Monreal
20160261ER

Project Description

This project seeks to prepare new bimetallic complexes that will provide valuable information about how actinide nitrides interact with other metals found in cladding material. Few molecular examples of actinide nitrides are available for study, owing to the difficulties in synthesis. Recent advances have provided routes to actinide azide and nitride complexes that expands the options for developing actinide nitride chemistry. The development of new molecular azide and nitride systems remains a major challenge in the field of actinide chemistry. Several questions now present themselves. What stoichiometric and catalytic reactivity might be achieved with terminal nitride linkages? Could molecular systems, such as the ones we propose to synthesize, constitute useful low-temperature precursors to actinide nitride materials? To answer these questions and more, an understanding of the electronic structure and chemical behavior of actinide nitride functional groups is needed. This proposal will do just that. This effort directly addresses the Los Alamos plutonium science research strategy to address our national security mission.

Baumann, D. O., K. A. Erickson, B. L. Scott, L. A. Silks, III, and J. L. Kiplinger. A Sterically Biased Unsymmetrical Azobenzene Derivative: Synthesis, Molecular Structure and ^{15}N NMR Spectroscopic Analysis of (E)-1-(2,6-diisopropylphenyl)-2-phenyldiazine. To appear in *Journal of Chemical Crystallography*.

Publications

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Monreal, M. J., L. A. Seaman, G. S. Goff, Michalczyk, D. E. Morris, B. L. Scott, and J. L. Kiplinger. New Twists and Turns for Actinide Chemistry: Organometallic Infinite Coordination Polymers of Thorium Diazide. 2016. *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*. **55** (11): 3631-3636.

Erickson, K. A., M. J. Monreal, A. G. Lichtscheidl, A. T. Nelson, B. L. Scott, D. E. Morris, and J. L. Kiplinger. Exploiting the Reactivity of Actinide Fluoride Bonds for the Synthesis and Characterization of a New Class of Bis(azide) Uranium Complexes. To appear in *Journal of Organometallic Chemistry*.

Tracking Microbial Effects on Water-Uptake and Productivity of Plants

Sanna Sevanto
20160373ER

Project Description

We use a combination of methods for non-invasive imaging and genomics to understand, for the first time, the complex interactions between the roots of plants and their microbial associates in the soil and how these influence plant survival. A successful project will deliver 1) world-class methods for studying plant-soil interactions, 2) in-vivo observations of the effects of mycorrhizal fungi on plant water uptake and drought responses, and 3) plant activity on root associates. We will combine unique capabilities to lead an emerging scientific field integrating fungal associates with plant functional responses. We will also develop non-invasive, high-resolution methods needed for understanding soil-plant interactions. Our results could revolutionize theories on plant stress responses and tolerance addressing significant gaps in our ability to predict plant productivity, vegetation changes and ecosystem-scale carbon cycling under changing climate.

Publications

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- Vesala, T., S. Sevanto, Y. Salmon, T. Gronholm, L. Lindfors, E. Juurola, E. Nikinmaa, I. Riipinen, P. Hari, M. Mencuccini, and T. Holta. Physical mechanism of reversed transpiration and enhanced water-use efficiency under plant water stress. 2017. *Frontiers in Plant Science*. x-x.
- Leigh, A., S. Sevanto, J. D. Close, and A. B. Nicotra. The influence of leaf size and shape on leaf thermal dynamics. Does theory hold up under field conditions?. 2017. *Plant, Cell and Environment*. **40**: 237-248.

Countering Pathogen Interference with Human Defenses

Geoffrey Waldo
20160054DR

Project Description

We will develop a detailed understanding of the way in which pathogens such as influenza virus interfere with human defenses designed to destroy them. This will provide a foundation for new therapeutics and diagnostics for influenza and other pathogens. Human cells can detect when they are infected by a virus or other pathogen and respond by activating machinery that destroys the infecting pathogen. To counter this, many pathogens such as influenza virus have evolved sophisticated methods to manipulate the control networks for these internal defense systems and evade destruction. In this project we will develop a detailed molecular understanding of how influenza virus interferes with "autophagy", a cellular defense system that can engulf and digest pathogens. Our project will create a foundation for the development of a broad range of next-generation therapeutics that block pathogen interference with human defenses and restore the natural ability of infected cells to destroy infecting pathogens. Our work will also provide a framework that can be extended to understand interference with host defenses by intracellular bacterial pathogens, such as Burkholderia, that are pertinent to defense threat reduction.

Using Therapeutic Bacteria to Treat Human Diseases

Jason Gans
20160340ER

Project Description

We aim to develop a technology that can be used to effectively treat gastrointestinal diseases using natural gut bacteria. We will demonstrate its utility by treating one of the deadliest diseases in the nation: Clostridium difficile. Clostridium difficile (C. diff.), is a major cause of gastrointestinal infections and is responsible for ~30,000 deaths every year in the U.S. alone. By the end of the project, we will demonstrate that a defined mixture of a few specific gut bacterial species can be used to effectively prevent and/or treat C. diff. infections in lab animals. The information gathered in this project will also help others better understand how equilibrium of species in a complex microbiome is established, and how it changes in response to various disturbances. This project will enable us to study the connection between the gut flora and several common inflammatory and autoimmune disorders, such as Crohn's disease, ulcerative colitis, cardiovascular disease, rheumatoid arthritis, etc.

Systems Out of Equilibrium

Angel Garcia
20160588DR

Project Description

This project addresses fluid systems out of equilibrium, such as porous media flows, thermal convection and stably-stratified shear flows, for applications in carbon sequestration, enhanced gas/oil recovery, and ocean dynamics. At the most fundamental level, we will investigate experimentally and numerically a range of fluid instabilities including low-Reynolds number porous media flows, thermal convection, and stably stratified shear flows. Hydrodynamic instability, turbulence, and mixing have application in ocean and atmospheric modeling and the characterization of astrophysical explosions and nuclear weapons physics.

Publications

- Olson Reichhardt, C., Y. Wang, Z. Xiao, W. Kwok, D. Ray, C. Reichhardt, and B. Janko. Pinning, flux diodes and ratchets for vortices interacting with conformal pinning arrays. 2017. *Physica C: Superconductivity and its Applications*. **533**: 148-153. <http://www.sciencedirect.com/science/article/pii/S0921453416300661>.
- Gerashchenko, S., and D. Livescu. Viscous effects on the Rayleigh-Taylor instability with background temperature gradient. 2016. *Physics of Plasmas (1994-present)*. **23** (7): 072121. <http://scitation.aip.org/content/aip/journal/pop/23/7/10.1063/1.4959810>.
- Kevrekidis, P. G., J. Cuevas-Maraver, A. Saxena, F. Cooper, and A. Khare. Interplay between parity-time symmetry, supersymmetry, and nonlinearity: An analytically tractable case example. 2015. *Physical Review E*. **92** (4): 042901. <http://link.aps.org/doi/10.1103/PhysRevE.92.042901>.
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Coupling Kinetic to Fluid Scales in Space and Laboratory Plasmas

Ari Le
20160647PRD2

Project Description

This project will perform advanced computer simulations to more accurately model two types of problems: (1) the interaction between the solar wind and the Earth's magnetosphere, and (2) the implosion of inertial fusion capsules. The fluid equations currently used to model plasmas are not always well justified. This is particularly true in critical regions such as shocks and thin boundary layers. In this project, we will demonstrate the feasibility of simulations that more accurately describe the entire complex system. We anticipate this project may improve our ability to more accurately model a variety of applications, including the space weather environment surrounding the Earth, and also the plasma dynamics within the fuel region of inertial fusion capsules.

Publications

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Boosting Algae Biomass for Biofuels with Plant Substrate Utilization

Amanda Barry
20170533ECR

Project Description

A Los Alamos priority is to secure energy solutions for clean energy and to mitigate the impacts of global energy demand growth. Optimizing algal growth through a mixotrophic (using light and carbon for growth) strategy utilizing cellulosic substrates and identifying potential high-value enzymes in biofuel production strains aligns with this focus and with DOE Bioenergy Technologies Office goals for improving algal biomass productivity. The proposed research will enable economical algal biofuel production by increasing algal biomass productivity and contribute to a stable domestic energy future.

Quantifying Covalency in Californium and the Other +3 Actinides

Samantha Schrell
20170663PRD1

Project Description

Identifying methods to measure subtle differences in M–Cl orbital mixing could have broad impact in virtually every technologically relevant area associated with the f-elements. This spans from isotope production to advanced nuclear fuel cycle development, plutonium sustainment, and the national nuclear security administration's (NNSA) missions in nuclear science. For example, many claims have rationalized unusual actinide behavior by invoking 5f-covalency in actinide-ligand bonding. As such, this project represents a leap forward for characterizing covalency in transplutonium metal-ligand bonding. We are excited at the opportunity to correlate the impact of covalency on the chemical and physical properties of important compounds and materials. Finally, these results have potential to serve as inspiration to strategically interrogate other actinide compounds in an effort to identify mechanisms to further enhance 5f- and 6d-contributions to covalent bonding.

Publications

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Prediction of Magnetic Properties of Actinide Complexes Using Ab Initio Methods

Ping Yang
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.

Laboratory Study of Fracturing and Hydraulic Conductivity through Heterogeneous Materials in Compressive Stress Environments

James Carey
20160642PRD1

Project Description

Our primary focus is to understand how mechanical damage (due to stress, temperature, fatigue, aging, chemical attack, etc.) to materials manifests as a changing permeability to fluids. These experiments will provide the first-ever study and x-ray imaging of fracture-fluid interactions at high-pressure and temperature and significantly advance our understanding of the consequences of fracture damage. Our work considers the behavior of heterogeneous materials with a particular application to high explosives. Analysis of the impacts of aging and deterioration of these materials are critical to DOE missions in nuclear weapons and explosives.

Publications

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

Patrick Chain
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.

Aromatic Actinide Metallacycles

Jaqueline Kiplinger
20170529ER

Project Description

The proposed research directly addresses the Los Alamos Plutonium Science and Research Strategy and Laboratory missions in Energy Security and Materials for the Future. A better understanding and control of covalency in the actinides will likely lead to new chemistries and reactivity trends that can be exploited to meet the needs of next-generation actinide science. This includes critical national priorities such as design of next-generation nuclear fuels, efficient separations in nuclear materials processing, a greater scientific basis for waste management, and materials stabilization issues relevant to weapons aging and corrosion processes. In essence, the insight we gain through this project could have widespread impact on designing stable aromatic and antiaromatic actinide complexes and to "turn-on" unique 5f-element electronic and optical phenomenon and reaction chemistry; thereby, directly addressing the BES grand challenge to Control Matter at the Most Basic Level of the Electron.

Publications

Pagano, J. K., K. A. Erickson, B. L. Scott, D. E. Morris, Waterman, and J. L. Kiplinger. Synthesis and characterization of a new and electronically unusual uranium metallacyclocumulene, $(C_5Me_5)_2U(\eta^4-1,2,3,4-Ph_4C_4Ph)$. 2017. *JOURNAL OF ORGANOMETALLIC CHEMISTRY*. **829**: 79-84.

Next-Generation Sea Level Predictions with Novel Ice Sheet Physics

Matthew Hoffman
20160608ECR

Project Description

This project will generate a robust capability of realistic basal physics for ice-sheet models developed and used by Los Alamos for improved sea level change predictions. Ice sheet basal sliding is the primary control on the flux of ice to the oceans; however, current predictions of sea level change from ice sheet models assume basal sliding will not change in the future, an assumption at odds with decades of research. Incorporating this crucial missing process will generate superior sea level predictions and a novel Earth System Modeling capability at Los Alamos. The impact of this work could be profound as sea-level change could potentially disrupt and displace coastal infrastructure and communities. Close to 150 million people live within 1 m of current sea level.

Publications

Hoffman, M. J., M. Perego, L. C. Andrews, S. F. Price, T. A. Neumann, J. V. Johnson, G. A. Catania, and M. P. Luthi. Widespread moulin formation during supraglacial lake drainages in Greenland. 2017. *Geophysical Research Letters*. **in press**.

Hoffman, M. J., L. C. Andrews, S. A. Price, G. A. Catania, T. A. Neumann, M. P. Luthi, Gulley, Ryser, R. L. Hawley, and Morriss. Greenland subglacial drainage evolution regulated by weakly connected regions of the bed. 2016. *NATURE COMMUNICATIONS*. **7**.

Measuring Messenger Ribonucleic Acid (mRNA) and Protein Content from Single Cells: Single Molecule Fluorescence In-Situ Hybridization on a Chip

James Werner
20170256ER

Project Description

This work is building the foundational tools to understand and detect the initial stages of bacterial versus viral infections. A biological attack is possible in both warfighter and civilian (e.g. terrorist) scenarios. The proper course of treatment of such attacks requires an understanding of the agent deployed (e.g. is it a toxin, or bacterial or viral in nature). This work is building the tools to understand how immune cells respond differently to bacterial versus viral infections at the single cell level. It will advance the state of the art in bioanalysis, measuring a suite of biomarkers (both proteins and nucleic acids) at the single cell level. We hypothesize that early events in disease diagnosis and progression will be clearer at the level of single cells, the level where infection starts and grows. This work will impact DOE/NNSA missions in warfighter and civilian protection from biological attacks, as well as helping with national needs in preventing the spread of infectious disease.

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).

Black Carbon Interactions with Radiation, Water & Ice: Laboratory Studies to Calibrate Arctic Climate Models

Manvendra Dubey
20160331ER

Project Description

Light-absorbing particles such as soot from forest fires or fossil fuel combustion and wind-generated mineral dust emitted in the atmosphere can be transported over long distances into the Arctic. There they can deposit onto snow and ice packs, darkening their surfaces and promoting melting by enhanced heating via light absorption. Current models treating these processes and effects are uncertain because they are idealized and not validated. In this project, we isolate and interrogate key processes and properties of these particles, including their light-absorbing power, scavenging by clouds and snowfall, and effects on the ice reflectivity in controlled laboratory experiments to test and refine the parameterizations used in models. Our results will increase confidence in quantifying the contributions of natural and anthropogenic light absorbing particles to the observed retreat of the Arctic sea ice and Greenland ice sheets.

Publications

Carrico, C., S. Bixler, A. C. Aiken, and M. K. Dubey. Low Hygroscopicity of Ambient Fresh Carbonaceous Aerosols from Pyrotechnics Smoke . Submitted to *Atmospheric Environment*.

Climate, Hydrology and Forest Disturbances in Southern and Western Watersheds

Katrina Bennett
20160654PRD2

Project Description

This project will develop a novel approach to quantifying changes in extreme events, with the goal of identifying critical watersheds where the greatest flooding and drought are anticipated to occur. The projected increase in frequency and intensity of billion-dollar weather and climate disasters, including severe storms, drought, and fire, is a significant domestic and global threat. We will develop a hydrologic model for the entire Colorado River basin (where key infrastructure and industry are located) that will be used to project future streamflow changes. One result will be a ranking of critical basins to determine the probability of future changes in extreme floods and droughts. This novel assessment of potentially destabilizing impacts will provide notable science results and new climate impact assessment technology to the national security community.

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Remediation Process Simulation-Optimization Under Complex Uncertainties

Velimir Vesselinov
20150711PRD2

Project Description

This project will advance an interval-fuzzy subsurface modeling system (IIFMS) for addressing interval and fuzzy uncertainties quantification (UQ) in modeling of contaminant fate and transport. Groundwater contamination can lead to adverse impacts and risks to society and the environment. Remediation costs are typically high and there is a big need for cost-effective strategies. Uncertainties are inherently associated with conceptualization and modeling of the contaminant fate, transport, and remediation process. Site remediation management is composed of various interconnected components that exhibit more complexities than its individual parts do. Such interconnections may lead to various complexities such as uncertainties in parameters and parameter relations, associated with dynamic and multi-objective features. We anticipate this work will be directly useful for generating more cost-effective remediation management strategies with improved efficiencies and increased robustness. The developed methods/models can also be applicable to other research areas where complicated uncertainties exist such as energy systems planning and surface water resources management.

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Building Full-scale Computational Models of Viruses

Sandrasegaram Gnanakaran
20160677PRD4

Project Description

Viruses are effectively ancient self-replicating microscopic machines that infect living organisms (i.e. humans, important food crops) and coerce them for the purpose of self-propagation. A deadly self-replicating, self-spreading entity could threaten public health, safety, and security. While many scientists study the spread of viruses at a population level using epidemiology, we focus on looking at the physically realistic computer model of a single virus (a single self-replicating machine) to gain insight about its behavior on the microscopic scale. The primary target outcome is biophysical insight into the behavior of enveloped viruses (especially HIV-1), which may reveal structural susceptibilities pertinent to vaccine, drug, and chemical neutralization efforts. This project has applications to all emerging viral threats, both natural and engineered, and aligns with the Laboratory's biosecurity mission. It directly supports the Science of Signatures science pillar, specifically in threat reduction and global health security. Unlike conventional bioweapon threats, a natural or engineered high-fatality pandemic is the greatest national security threat because of its global reach. This work will help solidify local efforts that seek to revolutionize DNA-sequence-based risk assessment of threats. Additionally, modeling of complex systems at the atomic scale builds our abilities for several other national security missions.

Mapping Cotranscriptional Assembly of the 30S Ribosomal Subunit to Illuminate Mechanisms of Antibiotic Interference

Peter Goodwin
20170156ER

Project Description

The ribosome, the primary machinery for protein synthesis in all living organisms, is an exquisitely complex, self-assembled multi-component structure, and as such, has become "the" model system for the study of self-assembly. Moreover, it is also the target for about 50 percent of clinical antibiotics. Our goal is a molecular-level understanding of the assembly of the 30S ribosomal subunit during transcription of its RNA scaffold. This new level of understanding will give unprecedented insight into mechanisms of antibiotic interference with ribosome assembly and identify new targets and assays for drug design. As such, this research supports Los Alamos missions to combat threats to U.S. health security, such as tuberculosis and methicillin-resistant staphylococcus aureus (MRSA), and provide defense against bio-threats such as anthrax and plague.

Publications

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Flow Cells for Scalable Energy Conversion and Storage

Rangachary Mukundan
20170046DR

Project Description

This project aims to develop low-cost, high-energy, high-power-density flow cell systems that have the potential to dramatically increase the amount of energy storage available in the US electrical grid. This increased availability of energy storage is expected to play a key role in increasing the penetration of renewable energies like wind and solar power. Specifically, this project utilizes a multi-pronged approach to develop novel chemistries and materials required to build high energy/power density non-aqueous flow battery systems. The development of such systems is in direct support of the DOE Office of Electricity Energy Storage program and is expected to have a positive impact on the national energy security mission.

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Multiscale Modeling of Biological Systems

Angel Garcia
20170509DR

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 DOE'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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Impacts of Extreme Space Weather Events on Power Grid Infrastructure: Physics-Based Modelling of Geomagnetically-Induced Currents (GICs) During Carrington-Class Geomagnetic Storms

Michael Henderson
20170047DR

Project Description

The project focuses on understanding the impacts that extreme space weather events may have on North-American power grid infrastructure. This will be accomplished by improving physics-based space weather models so that they can realistically simulate extreme events. The output of these improved codes will be used in power grid analysis tools to assess impacts on the ground. Aspects of the work can also be transitioned to the study of impacts on power grids of associated with nuclear weapons effects.

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Exploiting Quantum Interference to Control Ultracold Molecular Collisions

Brian Kendrick
20170221ER

Project Description

The proposed research will develop new fundamental capabilities in modeling and simulation for exploiting a newly discovered quantum interference mechanism to control the outcome of ultracold molecular collisions. The unprecedented dynamic range of this new mechanism provides the realization of a quantum switch capable of turning the collision outcome on or off. Thus, it opens up an entirely new domain of quantum control. The proposed work will lay the foundation for several transformative technological applications based on cold molecules, which is important to the DOE/NNSA missions in information science and technology and global security. These include: a new framework for realizing quantum computing, the development of sensors with unprecedented sensitivity, enable new tests of fundamental symmetries, improved astrophysics models of the interstellar medium/molecular clouds, and the synthesis of specific molecular species. The control of cold molecular collisions will also enable the formation of dense ensembles of cold molecules relevant for studying new exotic states of condensed matter and quantum phases.

Publications

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Atom-Efficient Upgrading of Bio-Derived Isopropanol/Acetone Mixtures

Andrew Sutton
20160671PRD3

Project Description

The project proposes to develop a chemical route to fuels and feedstocks using cheap abundant metal catalysts and low-energy input approaches to produce a cost-competitive process. We will take a bioderived building block and convert it to high-value chemicals and high-volume fuels. This dual-purpose approach allows for an agile strategy for replacing the whole barrel of oil with bioderived renewable sources. The result will be the development of catalyst systems to (1) efficiently dehydrogenate isopropanol to liberate dihydrogen and (2) upgrade the resulting acetone through self-condensation chemistry, targeting products with carbon chain lengths appropriate for fuel applications (C6 and greater).

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Critical Stress in Earth Crust

Paul Johnson
20170004DR

Project Description

A large earthquake in Cascadia or California would devastate the regional and potentially national economies. The primary national security challenge the 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 mid west. 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. Expected outcomes: The work is of 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.

Publications

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Breaking the "Curse of Dimensionality" for Boltzmann-like Systems

Gianmarco Manzini
20170207ER

Project Description

The goal of this project is to develop a new Information, Science and Technology capability for computer simulations of high-dimensional problems based on kinetic equations. A wide range of topics from computational science can benefit from its successful outcome, with potential mission-critical applications such as atmospheric and climate modeling and space weather simulation (global security/threat reduction) and magnetic fusion energy (energy security). This project will extend world-class numerical algorithms to high performance architectures, thus providing the DOE with unique computational capabilities useful for large proposals in computational co-design and extreme-scale solvers categories.

Publications

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- Manzini, G., and G. L. Delzanno. A discontinuous Galerkin-Hermite discretization of the Vlasov-Poisson system. 2017. *Los Alamos Technical Report (LA-UR-17-28541)*.
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Sensitive Optical Super-resolution Neuroimaging

Anatoly Efimov
20170249ER

Project Description

This project will produce advances in neural measurement and analysis technology, and enhance our ability to investigate, understand, and ultimately to emulate the function of the brain. Obvious applications include biomedical applications for diagnostics, therapeutics and prosthetic devices. Ultimately, such work will enable neural emulation: image understanding, natural language comprehension; closed loop control of motor function; and navigation in complex, dynamic environments. Similar processing techniques will generalize to problems outside of biological experience: analysis of hyperspectral imagery, detecting ultrasonic or electromagnetic signatures over wide frequency ranges; solution of ill-posed inverse problems; reasoning by inference or analogy based on very dense and complex data. Such applications have clear implications for national security responsibilities of the DoD and DoE.

Probing Ionosphere and Magnetosphere Connections with an Electron Gun

Gian Delzanno
20170423ER

Project Description

This project aims to remove the major obstacle (i.e. catastrophic spacecraft charging) to using high-power, relativistic electron beams for space applications relevant to science as well as to national security. In one potential application, known as radiation belt remediation, relativistic electron beams can be used to trigger plasma waves in the space environment. Waves can interact with the energetic particles of the environment and precipitate them at the poles, thus returning hazardous fluxes of energetic particles to more benign levels. Energetic particles in the near-Earth environment, the so-called 'killer electrons,' can cause catastrophic failure of our space infrastructure and pose a significant threat to national security. In another application, relativistic electron beams emitted from a magnetospheric spacecraft are used to probe ionosphere/magnetosphere connections with unprecedented accuracy. If successful, the long-term goals of the project are to (1) open up a new field of experimental space plasma physics based on electron beams, (2) enable the development of radiation belt remediation schemes to protect our space-based infrastructure, and (3) enable for the first time the resolution of several long-standing questions in ionospheric/magnetospheric physics.

Publications

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Bottom-up Chemical Synthesis of Large, Well-Defined, and Organo-Processable Nanographene-based Triarylamine for Optoelectronic Applications

Hung-Ju Yen
20140666PRD2

Project Description

Our project aims to synthesize processable nanographenes using multistep organic synthesis. We will then incorporate triarylamine into nanographenes to fabricate high-performance opto-electronics and highly efficient energy storage devices. Our proposed synthesis promises ways to control nanographenes (NG) with size-dependent band gap, optical absorptivity, and charge transfer functionality. If successful, this project will likely generate a new class of materials with emergent functionality previously not accessible through fabrication methods. The integration of functional NGs into clean-energy technologies could bridge the gap between basic research and commercialization of graphene-based energy devices. Further developing NG-based materials will strengthen our leadership role in NG research, which has strong ties to Laboratory mission in the areas of exotic materials and energy security.

Technical Outcomes

We used molecular synthesis to make unique carbon-based materials designed to meet the needs of a range of electronic applications, with perfect size and shape regularity, cheaply and at large scale. We created propeller-shaped molecules which feature three identical nanographene flakes joined at a central nitrogen atom, and showed that by tuning the structures by changing organic side chains at the periphery, it was possible to realize enhanced performance in lithium-ion batteries over ordinary graphite.

Publications

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Yen, H. J., C. Shan, L. Wang, P. Xu, M. Zhou, and H. L. Wang. Development of Conjugated Polymers for Memory Device Applications. 2017. *Polymers* . **9**: 25.

Yen, H. J., P. W. Liang, C. C. Chueh, Z. Yang, H. L. Wang, and A. K.-Y. Jen. Single Crystal Perovskite Powders for Large Grained Perovskite Solar Cells. 2016. *ACS Appl. Mater. Inter.*. **8** (23): 14513-14520. <http://pubs.acs.org/doi/abs/10.1021/acsami.6b02169>.

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Methane Coupling Chemistry Promoted by Catalysts Containing Inexpensive Metals

John Gordon
20150454ER

Project Description

Natural gas is comprised 75-90% of methane. As such, this molecule is one of the most abundant hydrocarbons on the planet; yet, current methodologies for the conversion of methane into commodity chemicals or fuels more amenable to transportation, storage, and use either depend upon high-energy input or on toxic/rare metals. We propose to use molecular catalysts to convert methane into ethane under mild conditions. The primary result from successful completion of this project will be experimental demonstration of each of the steps along the metal-dimer-catalyzed pathway for conversion of methane into ethane. Ethane a precursor to ethylene, a valuable chemical feedstock used in the production of important commodity chemicals that include polyethylene, surfactants, detergents, alcohols and others.

Technical Outcomes

The project initially explored the use of dimeric manganese complexes to couple hydrocarbon fragments (the ideal one being coupling methane units to make ethane). Based on subsequent computations, the project re-explored a more promising line – a monomeric manganese system. Evidence to this point, under manipulation of spin state, indicates success in coupling hydrocarbon fragments. This project added to the Laboratory's repertoire of bonding activation/forming chemistries, as well as expertise in chemistry for energy applications.

Climate Correlates of Tree Mortality

Chonggang Xu
20150744PRD3

Project Description

The work is focused on compiling and analyzing existing forest inventory network data from throughout the pan-tropics to determine the patterns and causes of forest mortality and survival in this important global carbon sink. The overall technical goals of this project are to document if, when, and where forest mortality is accelerating (or decelerating) pan-tropically, to understand the drivers, e.g. climate, and traits of the trees that are associated with survival and mortality, and to provide these results to Los Alamos, DOE, and international modelers that desperately need this information to improve predictions of the future pan-tropical forest carbon sink. The impact will be on the ecology, climate change, and modeling fields.

McDowell, and Sean M. McMahon. Separation of woody plants# drought and shade survival strategies: revisiting desiccation tolerance and avoidance. 2017. *Nature Ecology and Evolution*. In Review.

Technical Outcomes

Across the tropics, we found that species were classifiable into four “survival modes” that (1) explain life-history strategies shaping the terrestrial forest ecosystem carbon-cycle budget and (2) display the full range of life forms in the forest. Frequently collected traits, such as wood density, leaf mass per area and seed mass, were not generally predictive of these survival modes, suggesting poor alignment between these traits and survival strategies across tropical forests.

Publications

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Climate Impacts: Capturing Feedbacks and Adaptation in Coevolving Systems

John Moulton
20170614ER

Project Description

The potential impact of environmental disturbances, such as drought, flooding, extreme storms, and sea level rise, on infrastructure is a critical challenge for national and global security. Moreover, stakeholders have recognized the importance of the coupling and feedbacks between sectors (e.g., energy use, electrical infrastructure, water distribution) and natural systems (e.g., surface-water, groundwater, and wetland evolution) on decisions and planning. This multifaceted problem can only be addressed through the development of flexible workflow tools that enable a range of analyses and assessments, while supporting the development and use of sector models with a range of complexity and coupling characteristics. To explore the design of these workflow tools and sector models, scenarios involving natural system impacts on a representative site, the Delaware Estuary, are used. This foundational work is leading to the development of flexible cloud-based workflow tools that will be directly accessible to stakeholders and that can leverage extensive DOE high performance computing resources, as well as cloud-based computing resources. These advances have the potential to impact a wide range of DOE programs, including the grid modernization initiative, contaminant remediation and water resource management, the energy-water nexus and integration with the National Oceanic and Atmospheric Administration National Water Model initiatives.

investments produced better resilience vs. cost trade-offs than traditional strategies.

Technical Outcomes

The Delaware Estuary was identified as a data-rich site with transferable characteristics, and was used to develop a coastline erosion scenario that highlights natural system impacts on infrastructure. Specifically, a vulnerability analysis of the power grid was performed with, and without erosion, showing a significant change in the spatial locations of damaged assets. In addition, optimization over sequences of infrastructure hardening

Development of pH Responsive Protein Switches to Regulate Energy Capture and Conversion Processes in Photosynthesis

Richard Sayre
20150322ER

Project Description

We will design and develop advanced photosynthetic light harvesting complexes containing pH-sensitive protein conformational switches that more rapidly respond to high light stress, improving overall photosynthetic efficiency. Our overall objective is to develop novel pH-regulated protein conformational switches that will accelerate the dissipation of excess energy harvested by the photosynthetic antenna systems so as to reduce photodamage and increase biomass productivity. To achieve these objectives we will apply theoretical approaches to characterize energy transfer pathways, protein modeling studies to design switches, and biotechnology and biophysical approaches to develop and test the products. The targeted focus area for this proposal is sustainable production of clean energy.

Technical Outcomes

We have predicted that chlorophyll excited states generated within the CP29 photosystem II light harvesting protein chromophores have multiple pathways for deexcitation. We have demonstrated that CP29 transgenics with reduced CP29 levels have substantial reductions in non-photochemical quenching (NPQ). Site directed mutation at position Y175K which was predicted to alter the CP29 protein structure in a pH-dependent manner has been shown to impact NPQ processes enhancing overall photosynthetic efficiency by increasing NPQ yield by two-fold.

Publications

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Fighting Back Against Pathogens: Discovery and Validation of Novel Drug Targets

Ricardo Marti-Arbona
20150080ER

Project Description

This project develops the technology to define novel protein targets for new drug chemotypes effective against antimicrobial resistance (AMR) pathogens, especially those with multiple antibiotic resistance. We will focus the initial discovery and validation of novel drug targets in Burkholderia because of its wide resistance to antibiotic therapies, high mortality, and potential use as biological warfare agent. We will design, validate and apply RNA-based inducible modular regulatory elements to post-transcriptionally down regulate expression of 312 protein-encoding genes that are predicted to be critical to pathogen's survival and AMR, thus inactivating them. This will validate their usefulness as antimicrobial drug targets.

Technical Outcomes

We have developed a novel systematic approach to discover new ways to defeat multiple drug resistant (MDR) mechanisms in human pathogens. We use RNA-based Inducible Modular Regulatory Elements (IMREs) to mimic the antimicrobial effects of antibiotics. IMREs post-transcriptionally switch OFF the expression of 'putative' drug targets. IMREs are not antibiotics, but by mimicking the antibiotic's action, they identify essential proteins/genes that could be targeted for the production of novel drug chemotypes effective against MDR pathogens.

SHIELDS: Space Hazards Induced near Earth by Large Dynamic Storms - Understanding, Modeling, Predicting

Vania Jordanova
20150033DR

Project Description

Using a new, system-level approach, this project aims to provide transformative understanding of the mechanisms that drive disturbed geomagnetic conditions. This is critically needed so that we can accurately predict geomagnetic conditions and prevent damages to technological systems in space. Our national efforts in nuclear nonproliferation depend in many ways on our satellite sensing systems. Many of the nation's civilian and military space assets operate in the inner magnetosphere, an extremely hazardous region of space causing satellite failures and anomalies. The ability to reliably distinguish between various modes of failure is very important in anomaly resolution and forensics and may be used in decision-making exercises at the highest levels. This project will develop a new capability, the Space Hazards Induced near Earth by Large Dynamic Storms (SHIELDS) framework, to understand, model, and predict the spacecraft Surface Charging Environment, which is one of the most important space weather hazards.

Technical Outcomes

We developed SHIELDS, an end-to-end modeling capability of plasma behavior in the Earth's magnetosphere and its potentially catastrophic impact on space assets like satellites. Driven by solar inputs, it employs multiscale modeling and assimilates satellite observational data, demonstrating an order of magnitude improvement in the specification of the near-Earth space environment. SHIELDS is a new software platform that can provide warnings about an hour before a solar storm strikes, enabling protective actions to prevent damage.

Publications

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Global Tree Mortality Prediction Based on Hydraulic Function Failure

Chonggang Xu
20150030ER

Project Description

We propose to develop and evaluate the world's first global model of plant hydraulic function failure within a DOE-sponsored Earth System Model, aimed to better predict tree mortality under drought. The most important outcome of this project is a fully evaluated plant hydraulic function failure model at the global scale. Using this evaluated model, we will obtain drought-caused carbon loss in the past and for the future. Our laboratory measurements will provide a suite of complete datasets necessary for understanding plant hydraulics at the global scale, and our pattern-recognition approach will provide the first drought-caused tree mortality dataset for model evaluations at the global scale. Finally, we will quantify the relative importance of insects versus hydraulic failure as causes of drought-induced disturbances for different regions of the world.

Technical Outcomes

This project enabled the development of two critical models for prediction of tree mortality: a plant hydrodynamic model and a mountain pine beetle population model. The project also generated hydraulic trait data for model parameterizations and mortality data attributed to different agents for model evaluations. These model developments and data position the Laboratory to study vegetation responses and feedbacks to extreme climate events that link to national security.

Publications

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Characterizing Irregular Flows and Mass Transport in Microscopic Pore Spaces

Jeffrey Hyman
20150763PRD4

Project Description

Characterizing the influence of rock geometry on fluid flow provides needed insights to subsurface energy extraction and environmental stewardship. This project aims to determine the influence of pore structure on flow and transport, which will increase our ability to extract the next generation of fuel as well as advance the study of groundwater flow and transport, the disposal of used nuclear fuel, filter and textile design, and medical applications including the delivery of drugs to tumors. It also aims to increase the efficiency of the Immersed Boundary methodology. Lastly, it will improve understanding of the effects of fluid-gas interactions in the pore spaces, and their effect on the macroscopic flow. The developed computational toolbox will be applied to discrete fracture networks and lattice Boltzmann simulations. Characterizing fluid flow in porous media and controlling it is critical for the energy security mission.

Technical Outcomes

This project developed and advanced a particle tracking framework that can be applied to subsurface transport simulations ranging in scale from nano-meters to kilometers. We focused on direct numerical simulation of flow and mass transport through microscopic pore geometries and kilometer scale fracture networks where we linked the highly variable fluid velocity fields therein with upscaled mass transport properties including transport times and mixing.

Publications

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Toward a Coupled Multi-physics Modeling Framework for Induced Seismicity

Satish Karra
20150693ECR

Project Description

We aim to develop a new physics-based framework for induced seismicity that couples the traditionally separate fields of geomechanics and hydrology, and forms a basis for next-generation forecasting tools for induced seismicity modeling. The coupling will be achieved through the use of innovative new fracture-permeability damage relationships that describe flow changes by as much four orders of magnitude in the fractured zone around a fault rupture. The framework uses recent advancements in two high-performance computing simulators: PFLOTRAN for subsurface flow and QK3 for fault dynamics. The methodology will have wide utility for industry, academic and government partners in carbon sequestration, waste water injection and enhanced geothermal systems.

Technical Outcomes

A coupled flow-geomechanics framework was developed that evaluates the changes in the state of stress due to fluid injection/production as well as updates the hydrological properties such as porosity and permeability due to evolution of the state of stress. The state of stress evaluated through this framework can be used to identify if a fault has failed due to injection-related activity. Fault slip can be calculated with this framework for a fault that has failed.

Publications

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Fundamental Actinium Science In Search of Radiotherapeutics

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20150575ER

Project Description

We propose to investigate the fundamental properties of the radioactive element actinium. This relatively unstudied element is extremely promising for the treatment of cancer, and these studies will enable research towards clinical application. The proposed work will launch, for the first time, a comprehensive investigation of the chemical and electronic properties of the element actinium in support of rational design of actinium ligands for medical use. The chemical hardness, coordination number, and covalency of actinium ions in solution will be determined. An improved understanding of the fundamental chemistry of actinium is essential to the clinical use of actinium-225 for the therapeutic treatment of disease, in particular malignant disease. The nature of the facilities required to produce large amounts of actinium-225 ensures that only domestic facilities currently operated by the Department of Energy Office of Science have the capability to meet anticipated research demand for the isotope, if it can be shown functional in viable clinical trials.

Technical Outcomes

From this project, new methods for purification of Ac-227 and Ac-225 have been developed. Spectroscopic methods for highly radioactive yet minute masses of Ac-225 have been established, including UV-Vis spectroscopy, as well as the first ever use of EXAFS and NMR for characterization of actinium compounds. The first determinations of actinium-ligand bond distances have been made, including characterization of the actinium aquo species, that will inform future efforts towards clinical application of this important element.

Publications

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Critical Watersheds: Climate Change, Tipping Points, and Water Security Impacts

Richard Middleton
20150397DR

Project Description

The overarching goal of this project is to develop the science and modeling capabilities to predict and quantify climate impacts on critical watersheds and water supply. This will have a potentially transformative impact on our understanding of climate change and the energy-water nexus (EWN) and our ability to mitigate and adapt to climate change. Specifically, we are developing a new understanding of the interaction and feedbacks between climate change and extreme events, climate-driven disturbances such as wildfire, drought and forest mortality, hydrology, and water for the EWN. The project directly addresses the energy security and environment missions, with anticipated substantial contributions to the DOE applied energy and science programs.

Technical Outcomes

This project resulted in new science and capabilities. There is new understanding of feedbacks between climate-driven disturbances, ecosystems, and hydrology across multiple spatiotemporal scales, ranging from meters and seconds for individual storms in small watersheds, to regional hydrology across the Colorado River basin, to global drought through the 21st century. New capabilities include next-generation simulation tools to rapidly model wildfire behavior (QUIC-Fire; approximately a million times faster than previous models) and coupled surface-subsurface hydrology (ATS).

Publications

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Ocean Acidification Over the Last 13,000 Years

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20150242ER

Project Description

This project will reconstruct oceanic pH, temperature, oxygen and salinity levels of current (last 1000 years) and historic (11-12.5 kyrbp) periods to determine anthropogenic and upwelling strength impacts on ocean chemistry. We will also determine biological response to these chemical changes and predict the impact to fisheries, commerce, transportation, and energy infrastructures (cement in the oceans). This program will also advance the Laboratory's Secondary Ion Mass Spectrometer (SIMS) analysis capabilities and methodologies to measure few-micron, multiple elemental, isotopic signatures on mixed/heterogeneous materials. This will advance the instrument in its use on nuclear, particle, explosive, biological, chemical materials.

Technical Outcomes

Climate can impact global oceans through increased sea surface temperature (SST), deoxygenation, and acidification impacting local ecosystems (fisheries, coral systems). In 2015-2017, the Laboratory partnered with UC Santa Cruz, U. Wisconsin-Madison, and Arizona State University to determine if over the last 33k years, coastal oceans have experienced chemistry similar to today and if this impacted biological communities. We found shifts in SST, nutrient and oxygen levels impacted benthic foraminifera (plankton) which can impact local fisheries.

Publications

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Enhanced Photosynthesis through Carbon Concentrating Mechanisms

Scott Twary
20150226ER

Project Description

Producing renewable biobased fuels from algae requires optimizing the economic sustainability of production systems. DOE has identified algae productivity as a major factor limiting achievement of economic goals. Algae growth is dependent on photosynthesis providing the carbon for growth and lipid production. The objectives of this research were to maximize photosynthetic productivity in an industrial biofuel algae. A biophysical carbon concentrating mechanism was engineered into the algae chloroplast through production of hybrid proteins. These lines grew better under carbon-dioxide limiting conditions, providing pathways for lowering costly inputs while increasing biomass productivity. Diagnostic tools were developed for evaluating carbon use efficiency. These tools will have broad applicability to assess both genetic and culture system improvements in multiple algae lines. Genetic analysis identified key genes contributing to carbon limitation responses providing novel targets for continued genetic engineering improvements towards creating a domesticated algae industrial crop. The outcomes of this work will advance DOE BETO programs towards achieving sustainable biofuels production.

Technical Outcomes

Hybrid RuBisCO proteins were engineered into *Nannochloropsis* algae resulting in increased growth under CO₂ limiting conditions. Isotope discrimination analysis diagnostic tools were used to characterize carbon assimilation dynamics and carbon use efficiency. Key genes were identified that regulate the carbon concentrating mechanisms in *Nannochloropsis* providing novel targets for continued engineering enhancements.

Publications

Zidenga, T., M. Teshima, G. Perkins, T. Rahn, S. Twary, and J. Heikoop. Carbon use efficiency diagnostics in *Nannochloropsis salina*. To appear in *Algal Research*.

Selective Extraction of Medically-Relevant Radionuclides from Proton-Irradiated Thorium Targets

Michael Fassbender
20160439ER

Project Description

This proposal explores the production and high-yield chemical isolation of medically relevant isotopes for potential cancer therapy applications. A set of promising isotopes will be generated via proton irradiation of thorium targets at the Los Alamos Isotope Production Facility and a battery of selective chemical extraction methods will be utilized for the development and optimization of integrated processes that isolate proposed isotopes from the target matrix in chemical form for subsequent medical use. Targeted radiotherapy will provide an alternative to surgical resection, chemotherapy, and external beam therapy strategies.

Nortier, E. R. Birnbaum, K. D. John, and M. E. Fassbender. Simultaneous Separation of Actinium and Radium Isotopes from a Proton Irradiated Thorium Matrix. 2017. *SCIENTIFIC REPORTS*. 7.

Technical Outcomes

Targeted Radiotherapy (TR) provides a means to kill cancers while leaving healthy tissue unperturbed. Actinium-225 is one TR radionuclide formed in proton irradiated thorium targets. Therapy radionuclides $^{225}/^{223}\text{Ra}$, ^{111}gAg and auger-electron emitting ^{103}mRh are also formed and can be isolated as byproducts. A parallel multinuclide separation method was developed in an effort to design of a flow sheet in which a systems engineering approach is used to ensure simultaneous production with highest quantity and quality.

Publications

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Advancing Regenerative Medicine with Trinity: Defining a New State-of-the-Art for Biomolecular Simulation

Karissa Sanbonmatsu
20150755ER

Project Description

We will study the atomistic details of cell division, a large-scale process critical for stem-cell programming and regenerative medicine. A wide range of degenerative diseases remain potential targets for stem cell therapy and regenerative medicine; yet, converting stem cells into the appropriate specialized cell type remains a mystery. Current efforts in regenerative medicine have been largely spearheaded by trial-and-error strategies. Cell division is one of the key processes, but the atomistic details of this large-scale process have never been studied. We will perform the first atomistic simulations of condensation of chromosome material from an extended state to a condensed state. This will define a new state-of-the-art in biomolecular simulation, in terms of the number of cores used in a single simulation. In addition, performing the large-scale simulations will build general capabilities for other applications in the area of enzyme optimization, nanoparticle clusters, and nanowires. The project is also directly related to understand how Anthrax infections alter host epigenetic programs.

Technical Outcomes

We constructed the first atomistic model of an entire gene locus, performing a molecular dynamics simulation approximately 10x larger than the largest-to-date of an intact biomolecular complex (1 billion atoms). By developing a unique fast Fourier transform (FFT), we obtained strong scaling past 500,000 cores for 1 billion atoms with the GENESIS code on the Trinity platform. This represents a significantly larger number of cores and threads than any calculation to date in the biosciences.

Publications

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Sensing Swarms for Environmental Threat Reconstruction

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20170648ER

Project Description

This project provides a method for reconstructing an environmental threat such as infectious agents, toxic chemicals, or dangerous radiation from location data and wearable sensors. In disaster and battlefield settings, the environment may contain toxic substances that cause sickness in first responders and soldiers for example. The methods we developed in this project and reconstruct the concentration of unknown threats based on location data from people that moved through that space. These methods open up the possibility of integrating opportunistic sensing into threat assessment. That is, any population of people carrying a GPS enabled device (such as a cell phone) can be thought of as an opportunistic sensing swarm. This project also provides methods for quantifying the uncertainty in our estimates that can allow for the deployment of additional static sensors to increase precision.

Technical Outcomes

We developed a method for quantifying and visualizing an environmental threat from a sensing swarm, that is an undirected network of sensors that move through a physical space. For example, a swarm could be a group of people with GPS enable cells phone, some of whom become sick. These methods are essential for integrating opportunistic sensing, i.e. sensing data that is incidentally collected from dynamic sensors, into threat reduction.

Signatures of Gene Editing for National Security Science

Scott Twary
20170676ER

Project Description

Genome editing technologies and tools are expanding allowing for greater ease of modifications and broader application across species. These technologies can be used to alter organisms normal pathogenicity or host range. Identification of emerging threats requires characterization of the genomic changes. The objectives of this project were to define unique genome modifications after CRISPR Cas9 editing. Human kidney cell lines expressing green fluorescent protein (GFP) were edited by Cas9 treatments. Dark cells lacking GFP expression were characterized for genome modifications. Specific targeted genome editing of the GFP gene resulted in insertions, deletions, and mutation break points significantly different than untreated cells. This distribution of genome changes resulted in a biological signature of Cas9 editing in this genome. Continued analysis of the entire genome will identify off-target changes effecting non-target genes identified by clusters of mutations not seen in untreated cells. These tools can be expanded and applied to analyze organisms for natural or directed genome changes.

Technical Outcomes

Human kidney cell lines expressing green fluorescent protein were edited by Cas9 treatments. Dark cells lacking GFP expression were characterized for genome modifications. Specific targeted genome editing of the GFP gene resulted in insertions, deletions, and mutation break points significantly different than untreated cells. This distribution of genome changes resulted in a biological signature of Cas9 editing in this genome.

Bayesian Information Gap Decision Analysis

Velimir Vesselinov
20140000PRD4

Project Description

Bayes theorem is a mathematical technique that provides a way to determine the likelihood of different models given some observed data; we will extend this methodology to provide a framework for making decisions on complex problems. This project will apply an innovative Bayesian Information-Gap (BIG) uncertainty quantification (UQ) framework to a groundwater remediation scenario. BIG UQ is capable of informing scientifically defensible and robust decisions in the presence of severe uncertainties. Groundwater contamination is an important national problem with over \$100 billion dollars in liabilities including around \$20 billion within the DOE complex. A substantial challenge in groundwater remediation scenarios is to select between a variety of site characterization efforts and remediation options. This framework will provide insight into the value of different characterization efforts, inform the transition from studying the problem to solving the problem, and help select the best solution to the problem.

Technical Outcomes

This project developed methods and tools for making scientifically-defensible decisions in the context of severe uncertainty with a focus on decisions in groundwater contamination problems. The work led to a number of peer-reviewed publications as well as open-source software tools that are part of the Model Analysis & Decision Support (MADS) framework (<https://github.com/madsjulia/Mads.jl>). The methods and tools are currently being utilized in the Laboratory's environmental programs and work with external partners and collaborators.

Publications

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Ab Initio Modeling of Organometal Halide Perovskites for Photovoltaic Applications

Sergei Tretiak
20150758PRD3

Project Description

This work will aid in the design of organic-inorganic perovskite solar cells, providing valuable results to guide the design of future solar cell devices. The need for an affordable, clean, and abundant source of energy has generated large amounts of research in a variety of solution processed organic and hybrid organic-inorganic solar cells. A relative newcomer to the field of solution-processed photovoltaics is the lead halide perovskite solar cell. Using state-of-the-art computational techniques, we will characterize charge dynamics at the interface of perovskites in order to aid in materials design and device engineering.

Technical Outcomes

In 2011, the perovskite MAPbI₃ was discovered to have excellent properties for solar cell devices. While improvements to perovskite device efficiency happened rapidly, progress on perovskite device stability was more challenging. This project helped establish that photodegradation causes an accumulation of static charges known as small polarons. This phenomena can be mitigated by substituting the constituent species in the perovskite material. Also, it was found that two-dimensional perovskites have additional channels of manipulation.

Publications

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Access to Industrially Important Optically Active beta-X-alcohols via Direct Enantioselective Ester Hydrogenation

Pavel Dub
20140672PRD2

Project Description

Chiral catalysts are of pivotal importance for the production of many thousands of materials and products in the field of fine chemicals. Recent progress in science and technology demands more powerful and sophisticated catalysts bearing tunable functions. Asymmetric hydrogenation provides a powerful way to produce a wide range of enantio-enriched compounds without generating waste byproducts that traditional reductants might. This work will thus focus on developing new, well-defined, chiral bifunctional molecular catalysts via environmentally benign processes. Success in this chemistry could result in new approaches to polymers and materials synthesis for application to energy and bio security missions.

Technical Outcomes

This project developed a next generation of ligands and molecular catalysts for the mild single-phase hydrogenation of bio-renewable carbonyl containing functionalities into high-value intermediates. The project resulted in the series of new and novel ligands and efficient molecular catalysts including the ones with unique structures. A patent application was submitted based on results. Some of the ligands/catalysts are soon to be commercially available from a commercial supplier.

Publications

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Development of a Continuous Flow Reactor for the Conversion of Biomass Hydrolysates to Fuels and Feedstocks

Andrew Sutton
20160095ER

Project Description

We aim to make biofuels and renewable chemicals in low temperature, low pressure reactors using cheap catalysts to supplant our reliance on non-renewable fossil sources. The results of this research will be the characterization of the biomass catalytic upgrading process as a function of reaction engineering variables and reactor operating conditions. In addition, these results will be used to establish a process flow-sheet and preliminary economic analysis. The overall goal will be to produce mL quantities of fuel or fuel additive for future engine testing. This work directly supports our mission in energy security and will benefit defense applications.

Technical Outcomes

This project has enabled us to translate these batch reactions to fully heterogeneous 3-phase (liquid, gas, solid) continuous flow reactors and move to non-precious metal catalyst to achieve 100 fold improvement in reaction rates (from 14 hours to 10 minutes) with complete selectivity to the target products. This project resulted in a patent application.

Publications

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Petabyte-Scale Computational Analyses of Genomic Data to Elucidate Aging Mechanisms

Ludmil Alexandrov
20140670PRD2

Project Description

This project seeks to overcome some of the technical challenges associated with “big data,” which is pertinent to a number of national security applications. Large amounts of genomic data will be analyzed with the goal of identifying signatures of aging. The expected outcome is an in-depth characterization of the genetic changes that occur with age and the mutational processes responsible for these changes, which will have far-reaching implications for human health. The planned analyses will encompass roughly 25 petabytes of data and involve the use of advanced methods of multivariate statistics, novel method development, and new approaches to the use of computational resources to solve big-data problems. In overcoming the technical challenges of the proposed work, we will establish a “big data” science capability at Los Alamos that can be applied to diverse problems.

Technical Outcomes

We developed computational pipelines capable of processing petabyte scale cancer genomics data. Analyses of these data revealed no mutational signatures associated with cancer development and human aging—our main project goal. However, we were successful in gaining a variety of insights into cancer from our analyses.

Publications

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Linking Scaling and Mortality Theory to Understand Climate Impacts on Vegetation

Cathy Wilson
20140685PRD4

Project Description

Worldwide increases in temperature and drought have been associated with reduced growth and increased mortality of plants, but accurately predicting such responses is limited by a lack of process-based theory linking climate and whole-plant physiology. A promising way forward is metabolic scaling theory, which proposes that physiologic rates from cells to the globe are ultimately governed by rates of resource distribution through vascular networks and kinetics of resource utilization in metabolic reactions. This research will integrate for the first time the key mechanisms governing acquisition, distribution, and utilization of metabolic resources by plants. The result will be a general, process-based theory for understanding and predicting climate change effects on plant performance at multiple scales. This theory will significantly improve our ability to predict future vegetation dynamics and their feedbacks to climate.

Technical Outcomes

Dr. Michaletz developed and tested a new Metabolic Scaling Theory (MST) for predicting climate change effects on plant function from individuals to global scales. The MST includes physical processes of vascular network hydraulics, leaf heat transfer, and leaf photosynthesis, which together control the acquisition rates of key metabolic resources in plants. The Theory was evaluated with data from two DOE water and temperature manipulation experiments and the new DOE Next Generation Ecosystem Experiment-Tropics.

Publications

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Information Science and Technology

Assimilation Algorithms for Data Fusion in Large-scale Non-linear Dynamical Systems

Humberto Godinez Vazquez
20160599ECR

Project Description

Complex dynamical systems, such as space weather, climate, and energy grids, are plagued by noise and uncertainty, which severely hampers their accurate forecasting. Using recent mathematical breakthroughs we will significantly reduce forecasting error. We will develop a new method that greatly enhances the efficiency of assimilating data into large-scale models while still preserving the nonlinear dynamics. It will initially be tested on a 2D shallow water model, followed by a realistic space weather model. We will implement our methodology to a magnetohydrodynamic model, to correctly specify Earth's magnetosphere. We will study its applicability to the Los Alamos space infrastructure, which will add critical forecasting to space awareness capabilities. A software library with the relevant assimilation method will be produced, tested, and released.

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Publications

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Neuromorphic Memcomputing via Interacting Nanomagnets

Francesco Caravelli
20170660PRD1

Project Description

The brain is estimated to perform up to $E+16$ operations per second. To perform at the same level, a supercomputer would consume circa $E+15$ Watts, whereas the brain consumes only 25 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.

Publications

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Large-Scale Nonlinear Optimization via Cloud Computing

Carleton Coffrin
20170574ECR

Project Description

The proposed work will develop a world-leading algorithm for large-scale nonlinear distributed optimization. This capability will advance our understanding of the fundamental challenges inherent in optimizing infrastructure systems, large-scale machine learning, and dynamical systems. The resulting general-purpose nonlinear optimization software is applicable to a wide-range of large-scale simulation and optimization tasks faced by the Department of Energy and others.

Hybrid Quantum-Classical Computing

Rolando Somma
20160069DR

Project Description

This project will investigate the potential of hybrid quantum-classical computing to deliver significant gains in computing speed. Our findings will play a paramount role in the design of future computing architectures. Hybrid quantum-classical computing (HQCC) provides the potential for orders-of-magnitude faster computation than is possible by today's computers. The main goal is to investigate the computing power of physically realizable quantum annealers, exemplified by a D-Wave device. HQCC will deliver powerful algorithms for optimization, with potential applications that range from materials science to national security. These algorithms will be implemented in an available D-Wave quantum annealer and on conventional computers, using advanced numerical methods that simulate quantum annealers. HQCC will also conduct quantum annealing experiments, which will allow us to study the physical phenomena that can impact the efficiency of quantum annealers at very large scales.

Publications

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A Multiscale, Non-stochastic Approach to Model Collisions in Particle Systems

Luis Chacon
20160448ER

Project Description

This project aims at developing a noise-free collisional particle treatment for physical systems of relevance to the Los Alamos mission. This research will enable high-fidelity simulations with far fewer computational resources than ever before. We will demonstrate the feasibility, accuracy, and efficiency of deterministic (vs. stochastic) particle collisional treatments in two applications of relevance: thermal radiative transfer and semi-collisional plasmas. The successful conclusion of the research proposed in this project will enable unprecedented fidelity in the modeling of these two physical systems with far fewer computational resources, thus opening a new computational frontier. The methods proposed here will also conform naturally to modern architectures such as the Trinity supercomputer, thus opening the possibility of high utilization of modern computing architectures. The algorithms stemming from this research, once successfully demonstrated, will impact a variety of mission spaces including energy security and nuclear security defense.

Publications

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- Park, H., L. Chacon, A. Matsekh, and G. Chen. A multi group scale-bridging deterministic particle solver for time-dependent thermal radiative transfer problems. Submitted to *Journal of Computational Physics*.

Efficient Exploration of High-Dimensional Model Structural Uncertainties

Nathan Urban
20160189ER

Project Description

We propose to develop efficient techniques to measure uncertainties in computer model predictions that exist due to different choices of physical approximations. The goal is to automatically explore the computer-simulation uncertainties without having to rewrite and re-run the model for each new approximation. These uncertainties can be pervasive in many fields, such as climate science, fluid dynamics, material science, etc. We will test new automated uncertainty quantification techniques on a series of idealized problems from geophysical fluid dynamics to test the validity of the methods. If successful, this would revolutionize how computer model structural uncertainties are quantified. Currently, this work is done slowly, by hand, exploring only a narrow range of possible uncertainties.

Global Optimization Methods for Structural Bioinformatics

Hristo Djidjev
20160317ER

Project Description

This project develops algorithms for predicting the 3D structure of proteins, which helps understand their function. The results of this project can lead to a breakthrough in drug design and finding cures for diseases such as Parkinson's and cancer. The proposed work will result in algorithms and tools for structural bioinformatics, focusing on predicting the structural alignment of proteins. We will restrict our focus to versions of those problems that can be modeled as quadratically constrained quadratic problems. Such problems include multi-component protein assembly, side-chain positioning, inverse folding, and multiple structural alignment. In order to validate our models and test the efficiency of our algorithms, we will use data banks such as the Protein Data Bank (PDB). While this proposal focuses on bioinformatics, the global optimization framework that we develop could also impact the Laboratory's information science and technology capability and has the potential to be extended and applied to other areas such as cybersecurity and co-design.

Publications

Guillaume Julien Chapuis. , and Hristo Nikolov Djidjev. Parallel Computation of Betweenness Centrality for Large Planar Graphs. 2016. *SIAM Workshop on Network Science (NS16)*. <http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-16-21526>.

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Controlling Quantum Information by Quantum Correlations

Wojciech Zurek
20170675PRD2

Project Description

The main goal of the project is to design protocols to control quantum systems, which outperform any known classical strategies. In particular, we plan to determine how quantum correlations can decrease the time and the energy for driving a system into the optimal state to run a quantum computation. We will design experimental demonstrations of quantum correlation-boosted control, implementable e.g. in optical lattices and atom traps. The project will pave the way for achieving optimal control of complex quantum systems, which is essential to deliver scalable quantum technologies. The proposal fully aligns with the Laboratory's commitment to be a strong player in developing quantum science and technologies, which has been recognized as a strategic priority by the National Science and Technology Council and the National Security Agency. Quantum devices are expected to dramatically change big data processing, solving computational problems beyond the capability of the best classical machines, and leading to innovative solutions in critical sectors as environmental sustainability, energy provision, and national security.

Publications

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Susa, C. E., and D. Girolami. Weaving and neural complexity in symmetric quantum states. 2018. *Optics Communications*.

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Tensor Networks and Anyons: Novel Techniques for Novel Physics

Lukasz Cincio
20160643PRD2

Project Description

The main goal of the project is to create a scalable, numerical tool that will enable insights into two-dimensional quantum systems. In particular we plan to apply it to study topologically ordered phases and, more importantly, identify experimentally realizable systems that may serve as platforms for quantum computation. Our results will help in the design of quantum computers, which has immediate implications for national security. More generally, we anticipate that our tool will enable subsequent theoretical and experimental research.

Publications

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Hickey, , Cincio, Papic, and Paramakanti. Emergence of chiral spin liquids via quantum melting of noncoplanar magnetic orders. 2017. *PHYSICAL REVIEW B*. **96** (11).

Convolutional Compressive Sensing for Scientific Imaging

Cristina Garcia Cardona
20170549ECR

Project Description

Converting large amounts (terabytes) of observational data into meaningful information about the sample under study (morphology, composition, phase distribution, etc.) is extremely challenging. Inverse modeling is one of the analytical techniques that tries to facilitate the conversion of measurements into interpretable knowledge by formulating a mathematical model to explain the data and estimating the parameters of the model that best fit the observations. Ideally, the fewer measurements needed to characterize the sample, the greater the potential to maximize the performance and to reduce operation costs, since less time is required for experiment execution and less data has to be stored and processed. We are developing a novel inverse modeling technique that enables the accurate reconstruction of signals from incomplete sets of observations by learning a mathematical model that exploits intrinsic properties of the physically measured data (e.g. sparseness: few active components). Being able to assimilate information and extract knowledge from large experiments and to increase the performance (accuracy and speed) for sample reconstruction is crucial for the success of future facilities such as MaRIE and other DOE facilities producing high rates of imaging data.

Jialin Liu. , Cristina Garcia-Cardona, Brendt Wohlberg, and Wotao Yin. Online Convolutional Dictionary Learning. 2017. In *Proceedings of IEEE International Conference on Image Processing (ICIP)*.

Publications

Cristina Garcia-Cardona. , and Brendt Wohlberg. Subproblem Coupling in Convolutional Dictionary Learning. 2017. In *Proceedings of IEEE International Conference on Image Processing (ICIP)*.

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Jialin Liu. , Cristina Garcia-Cardona, Brendt Wohlberg, and Wotao Yin. Online Convolutional Dictionary Learning. 2017. *Submitted to SIAM Journal on Imaging Sciences*.

Cristina Garcia-Cardona. , and Brendt Wohlberg. Convolutional Dictionary Learning. 2017. *Submitted to IEEE Transactions on Computational Imaging*.

Real-Time, Real-World Time Series Forecasting Using Internet Data

Reid Priedhorsky
20160595ECR

Project Description

Tracking disease with internet searches and social media can improve public health response, but this field (despite wide reporting) has shown mixed success, due in part to a lack of theory and controlled experiments. The proposed work will make critical progress toward a deployed science of reliable disease forecasting with quantitative uncertainty, as well as in the broader data science of large-scale, real-world forecasting. While many of the individual tools are standard, their emergent behavior in a combined setting is novel. Deliverables include a mathematical description of the information pipeline that transforms human observations into actionable knowledge via internet systems; validation of this pipeline using controlled experiments in a simulated setting; validation of this pipeline in diverse real-world settings; and quantification of the value of internet data for disease forecasting. This work addresses the Laboratory's global security mission.

Publications

Ashlynn Rae Daughton. , Kelly Renee Moran, David Allen Osthus, and Reid Priedhorsky. Internet data sources for disease surveillance: Assessment of suitability. 2017. <http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-17-21519>.

Trace Elements in Martian Rocks and Soils as Observed by ChemCam in Gale Crater, Mars, and Preparation for LANL's Next Mars Mission

Roger Wiens
20160650PRD2

Project Description

This project will consist of performing calibrations of minor and trace elements for laser-induced breakdown spectroscopy (LIBS), expanding the capability of LIBS for space and ground missions. The rover will go to several regions that define the main goals of the mission, particularly a clay-rich region identified from orbit. Having better trace-element capabilities will be very helpful in the overall goals of the rover mission. LIBS can be applied in a wide variety of rugged environments, so it is potentially practical for detecting explosive residues, detecting transuranic elements and uranium isotope ratios, detecting contamination (e.g., Be, Pb), and even for making some medical detections.

Publications

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Real-time Adaptive Acceleration of Dynamic Experimental Science

James Ahrens
20170029DR

Project Description

This project aims to accelerate knowledge-to-discovery from experimental scientific facilities by combining computer and statistical science to produce an adaptive methodology and tool set that will analyze data and augment a scientist's decision-making so that the scientist can optimize experiments in real time. We will develop this capability in the context of dynamic compression experiments at advanced light sources, an area of core mission importance for Los Alamos and an area that is currently in the midst of substantial increases in the rate of data generation. This project will result in a data science focused information science and technology tool set that is optimized for and will revolutionize dynamic compression science experiments using X-ray user facilities. Our novel approach will strengthen national security by enabling scientific results from experimental facilities to be directly relevant to our stockpile stewardship mission.

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Sandberg, R. L. Tools for Real-time Adaptive Acceleration of Dynamic Compression Science at Light Sources. Presented at *2017 LCLS/SSRL User Meeting*. (Menlo Park, CA, 27-29 September 2017).

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Publications

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Dutta, S., J. Woodring, H. W. Shen, J. P. Chen, and J. Ahrens. Homogeneity guided probabilistic data summaries for analysis and visualization of large-scale data sets. To appear in *IEEE Pacific Visualization Symposium (PacificVis)*. (Seoul, South Korea, 18-21 Apr. 2017).

3D Structure from Drone and Stereo Video

Garrett Kenyon
20170155ER

Project Description

The main national security challenge this research addresses is the need to develop techniques that can learn useful representations from large, unlabeled datasets, such as drone video, infra-red "night-vision" video, etc. We adopt a biologically motivated approach to learning such representations by attempting to implement the self-organizing principles governing cortical development. Ultimately, we hope to enable intelligence and military analysts with the ability to annotate a relatively small number of examples of a given target in a particular video clip and to then search for that same target in additional clips.

Publications

Lundquist, S., M. Mitchell, and G. T. Kenyon. Sparse coding on stereo video for object detection. To appear in *NIPS*. (Long Beach, Dec 4-9, 2017). <http://https://arxiv.org/abs/1705.07144>.

Asynchronous Navier-Stokes Solver on 3D Unstructured Grids for the Exascale Era

Jozsef Bakosi
20170127ER

Project Description

The project pioneers computer science technology required to use the largest future computers in an energy-efficient fashion to simulate physics problems. While the project concentrates on hydrodynamics, our software design is prepared for future multi-physics simulations, e.g., coupling with reactions, radiation, electrodynamics, and magnetism among non-ideal multiple materials. With such vision pointing well beyond this project, we anticipate an impact on multiple Los Alamos and DOE/NNSA programs, including high-energy-density hydrodynamics, global security, astrophysics, as well as atmospheric, climate, and fusion energy sciences. If successful, this project will put Los Alamos at the forefront of exascale real-world fluid dynamics; furthermore, by delivering not just a mini application (that only mimics certain aspects of production software) but a production-like open-source code, it may provide a fully asynchronous extensible software infrastructure for Los Alamos mission.

Publications

Bakosi, J., R. Bird, C. Junghans, R. Pavel, J. Waltz, F. Gonzalez, and B. Rogers. Quinoa: Adaptive Computational Fluid Dynamics. Presented at *15th Annual Workshop on Charm ++ and its Applications*. (Urbana-Champaign, 17-19, Apr. 2017). <http://https://charm.cs.illinois.edu/workshops/charmWorkshop2017/program.php>.

Next Generation Image Processing and Analysis Algorithms for Persistent Sky Surveillance

Przemyslaw Wozniak
20170183ER

Project Description

In the 21st century, space has become a competitive arena that demands constant innovation to meet the nation's security goals. Custody of Resident Space Objects (RSO) requires persistent monitoring on a global scale to extract rare and subtle signatures of important state changes and maneuvers. Looking everywhere all the time is expensive and requires substantial investments in hardware deployed around the world. It is therefore critically important to develop sophisticated algorithms that can achieve more with less hardware. Accurate direct pixel-by-pixel image subtraction based on convolution is an essential tool for processing crowded sky surveillance images. Our key objective is to develop an effective regularization method to stabilize the convolution kernel while preserving the required flexibility. Another problem is source confusion, i.e. unreliable image segmentation and light attribution for faint sources. We will develop new source extraction and point-spread function recovery algorithms based on modern exemplar models. This will lead to a dramatic reduction in artifacts, allow a much cleaner extraction of important signatures, and enable robust selection of events of interest. Image processing algorithms developed by this project have a potential to significantly enhance the detection sensitivity and coverage of the imaging sensors used for space object tracking.

Optimization and Physics Inspired Machine Learning Approaches

Angel Garcia
20170508DR

Project Description

Physics Informed Machine Learning (PIML) merges cutting-edge computational and algorithmic ML tools with physical knowledge in the form of constraints, symmetries, and domain expertise regarding effective degrees of freedom. Our focus is to develop methodologies and algorithms for the optimization and control of power and infrastructure systems, automated model reduction and coarsening, and learning macro-scale models that capture relevant physics of micro-scale simulations. The resulting technologies are applicable to a wide range of mathematical structures that arise in practical applications related to control and operations of complex engineered network, such as natural gas and water systems.

Publications

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Parameter estimation in a thermoelastic composite problem via adjoint formulation and model reduction. 2017. *International Journal for Numerical Methods in Engineering*. **112** (6): 578-600. <http://onlinelibrary.wiley.com/doi/10.1002/nme.5530/abstract>.

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applications to distribution system of the power grid. 2017. In *2017 American Control Conference (ACC)*.p. 813.

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Development of Computational Methods for Large-Scale Simulations of Heavy Elements in Solution Environments

Enrique Batista
20170198ER

Project Description

A computational methodology that can simulate thousands of atoms in solutions containing heavy elements and nuclear products is much needed to use computers in the design of remediation approaches. Such a capability would find application immediately not only at Los Alamos but in other areas of DOE such as environmental management (EM), NNSA, NE, and other agencies. Currently such a simulation is impossible. This project plans to address the development of techniques for large-scale simulations of chemical processes involving nuclear materials. The success of this proposal will provide the Laboratory with a first-of-its-kind capability, allowing us to carry out realistic solution chemistry simulations with multiple components.

Computational algorithms for modeling non-adiabatic dynamics in molecular systems

Dima Mozyrsky
20170460ER

Project Description

Upon completion, this project will result in novel computational capabilities critical for understanding light-induced dynamics in many technologically relevant molecular systems and nanostructures. In particular our studies will boost our ability to model molecular dynamics that involves transitions between different electronic states in a molecule, which is the case, for example, when a molecule absorbs a photon (i.e. a quantum of electromagnetic radiation). Such physical processes are common in a multitude of situations of physical, chemical, biological and technological interest, ranging from light harvesting or photosynthesis to the physics of high-energetic materials (i.e., explosives). We believe that the numerical algorithms developed in the course of the project will enhance accuracy and thus our predictive power in modeling these materials and processes, which, in turn, will lead to further technological development and design of relevant materials and systems. Our new unique theoretical capability can immediately provide a substantial impact on a number of existing and future programs at Los Alamos and DOE.

Publications

Daligault, J., and D. Mozyrsky. Non-Adiabatic Quantum Molecular Dynamics with Detailed Balance. Submitted to *Physical Review Letters*.

High-Order Hydrodynamic Algorithms for Exascale Computing

Nathaniel Morgan
20170051DR

Project Description

The objective of the research is to improve hydrodynamics algorithms, which are of great importance to science-based prediction in programmatic applications. Hydrodynamic simulations at Los Alamos are regularly used to (1) design hydrodynamic experiments where many exceed a million dollars to execute, (2) aid understanding of experiments, (3), interpolate between different experiments, (4) estimate margins and uncertainties, (5) investigate high strain-rate deformation of metals, and (6) extrapolate experiments into regimes and scales that are not readily accessible. This research will likely positively impact many key Laboratory programs such as the Advanced Simulation and Computing (ASC) program and the DoD/DOE joint munitions program. Developing high-order algorithms is also beneficial to computational fluid dynamics (CFD) codes that are used at Los Alamos to simulate flows in such applications as internal combustion engines, casting of metal parts, and climate models. The results from this research effort could radically transform the computer simulation capabilities at Los Alamos and beyond.

Publications

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- Liu, X., N. R. Morgan, and D. E. Burton. A Lagrangian discontinuous Galerkin hydrodynamic method for 2D Cartesian and RZ axisymmetric coordinates. To appear in *2018 AIAA SciTech Forum*. (Kissimmee, Florida, 8-12, Jan. 2018).
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Advancing Predictive Capability for Brittle Failure Using Dynamic Graphs

Gowri Srinivasan
20170103DR

Project Description

This project addresses the failure of brittle materials and fluid flow through fractures in brittle materials, in applications of interest to global and national security. The former is a concern for weapons performance where it is critical to predict how fractures propagate in materials leading to damage and eventually failure. Our algorithms will predict failure times quicker and more accurately under a wide range of commonly encountered scenarios, which increases confidence in our predictions. We will also model how gases flow through fractured medium below the surface in the aftermath of a chemical or nuclear explosion. It is critical to detect the nature of explosions based on identifying gases such as Xenon that migrate upward to the atmosphere through fractures that already exist in natural formations and those created by the blast. Being able to detect these gases is of utmost importance to our Nuclear Nonproliferation programs. We will also predict failure times and patterns in the case of brittle materials, which is a phenomenon of importance in nuclear weapons performance. The Advanced Simulation and Computing (ASC) program will benefit from more accurate models to predict failure for various weapons performance scenarios.

Publications

- Srinivasan, G., J. D. Hyman, D. A. Osthus, B. A. Moore, D. O'Malley, S. Karra, E. Rougier, A. A. Hagberg, A. Hunter, and H. S. Viswanathan. Quantifying topological uncertainty in fractured systems using graph theory and machine learning . Submitted to *Nature Scientific Reports*.
- Valera, M., Z. Guo, P. Kelly, S. Matz, A. Cantu, A. G. Percus, J. D. Hyman, G. Srinivasan, and H. S. Viswanathan. Machine learning for graph-based representations of three-dimensional discrete fracture networks. To appear in *Computational Geosciences*.
- Osthus, D., H. Godinez, E. Rougier, and G. Srinivasan. Calibrating the stress-time curve of a combined finite-discrete element method to a split Hopkinson pressure bar experiment. Submitted to *International Journal of Rock Mechanics and Mining*.

- Miller, R. L., B. Moore, H. Viswanathan, and G. Srinivasan. Image analysis using convolutional neural networks for modeling fracture propagation. To appear in *IEEE International Conference on Data Mining (ICDM)*.(New Orleans, LA, 18 Nov, 2017).
- Hyman, J. D., and J. Jimenez-Martinez. Dispersion and mixing in three-dimensional fracture networks: nonlinear interplay between structural and hydraulic heterogeneity. Submitted to *Water Resources Research*.
- Djidjev, H., D. O'Malley, H. Viswanathan, J. D. Hyman, S. Karra, and G. Srinivasan. Learning on graphs for predictions of fracture propagation, flow and transport. 2017. In *2017 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*.(Orlando, June 2017). p. 1532–1539. Orlando: IEEE.
- Hickmann, K. S., J. D. Hyman, and G. Srinivasan. Efficient and robust classification of seismic data using nonlinear support vector machines. To appear in *Asilomar Conference on Signals, Systems, and Computers*.(Pacific Grove, CA, Oct 29 - Nov 1, 2017).
- Hyman, J. D., Hagberg, Srinivasan, Mohd-Yusof, and Viswanathan. Predictions of first passage times in sparse discrete fracture networks using graph-based reductions. 2017. *PHYSICAL REVIEW E*. **96** (1).

Microstructure Sensitive Radiation Effects

Laurent Capolungo
20170615ER

Project Description

Typical models transcribing the response and microstructure evolution of metals are weakly connected to materials chemistry. The novel hybrid model proposed will, for the first time, address this issue in the context of radiation-induced damage. In the long term, this work should yield a path towards materials selection for nuclear environments.

Publications

- Stewart, J., A. Kohnert, L. Capolungo, and R. Dingreville.
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A Polyhedral Outer-Approximation, Dynamic-Discretization Solver for Mixed-Integer Semi-Definite Programming (MISDP)

Russell Bent
20170201ER

Project Description

Analysis of critical infrastructure (electric power, 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, 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 modeling these systems. 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

- Wu, F., H. Nagarajan, A. Zlotnik, R. Sioshansi, and A. M. Rudkevich. Adaptive convex relaxations for Gas Pipeline Network Optimization. 2017. In *Proceedings of the American Control Conference*.(Seattle, 24-26 May, 2017). p. 4710. Seattle: IEEE.
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Coupled ALE-AMR for 3D Unstructured Grids

Jacob Waltz
20150414ER

Project Description

This project develops innovative approaches for the numerical modeling of high-speed material flows. We expect our research to lead to significant improvements in fidelity and computational efficiency for work related to NNSA defense programs, nonproliferation, and science campaigns. The impacts of these improvements will include faster responses to programmatic questions; increased population sizes for uncertainty quantification and other sensitivity studies; greater detail in discovery-scale simulations; and an enhanced ability to model realistic 3D features. Looking into the future, the advances in simulation capability that results from our research could apply to design of blast mitigation structures for urban environments, energetic disablement calculations of improvised explosive devices, anti-personnel and anti-structural analysis, high-resolution studies of mix and ignition in Inertial Confinement Fusion targets, and astrophysics.

Technical Outcomes

This project successfully developed and demonstrated advanced techniques for Arbitrary Lagrangian-Eulerian (ALE) mesh motion and the coupling of ALE with Adaptive Mesh Refinement (AMR).

Publications

Waltz, J., and J. Bakosi. Advances in coupled ALE-AMR for tetrahedral grids. Presented at *14th U.S. National Congress for Computational Mechanics*.(Montreal, Canada, 17-20 July 2017).

Waltz, J., J. Bakosi, and N. Morgan. A Helmholtz based approach for arbitrary Lagrangian-Eulerian mesh motion. Presented at *World Congress on Computational Mechanics*.(Seoul, South Korea, 25-29 Jul. 2016).

Bakosi, J., J. Waltz, and N. Morgan. Improved ALE Mesh Velocities for Complex Flows. 2017. *International Journal for Numerical Methods in Fluids*. 1-10.

Waltz, J., J. Bakosi, and N. R. Morgan. A coupled ALE-AMR approach for shock hydrodynamics on tetrahedral

grids. Presented at *United States National Congress on Computational Mechanics*.(San Diego, CA, 27-31 Jul 2015).

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Spatial and Extreme Value Processes for Bridging Micro- and Macro-Scales in Materials

Scott Vander Wiel
20150594ER

Project Description

We will develop theoretical, statistical models to account for spatially distributed extremes, and to efficiently summarize micro-scale information in a way suitable for use at the macro-scale. There is a demonstrated need for advancement in computational prediction of damage and failure in polycrystalline metallic materials, particularly for our weapons calculations. This is largely a result of inadequate physics and material statistics representation. This project is designed to address this shortcoming in how we represent such processes. We will demonstrate a viable approach for statistically characterizing micro-scale properties of a polycrystal, and using these properties to predict the material's strength and damage properties at a macro-scale, under some rather simple loading scenarios. We also expect this effort will illuminate promising new directions for analysis approaches that can bridge the micro- and macro-scales. In particular, we will seek new statistically rigorous representations of damage nucleation in polycrystalline materials.

Technical Outcomes

New statistical tools advance a capability relating macro-scale mechanical properties of a polycrystalline material to its heterogeneous micro-scale details. Our statistical model for multi-grain stress fields matches computations showing a tendency for elevated stress at grain boundaries, especially triple junctions, and correlated locations across grains. We also predict grain boundary stress from the eight degree of freedom grain boundary character (a normal vector and two crystallographic orientations.) Symmetrized hyper-spherical basis functions are a key enabler.

Publications

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Long-time Dynamics using Trajectory Splicing

Arthur Voter
20150557ER

Project Description

We are developing a novel way of simulating the evolution of materials through the concept of "trajectory splicing." We will develop the ParSplice method and deliver an implementation that is nominally exascale ready. This state of readiness will be validated through extensive simulations using our performance prediction approach. The design and parameter spaces will be thoroughly explored so as to be ready to adjust the implementation as novel architectures emerge. We will also deliver a thorough formal understanding of the method. Such a capability is invaluable to investigating the microstructural evolution of materials and understanding their performance in operation conditions.

Technical Outcomes

We developed a novel approach, parallel trajectory splicing (ParSplice) for achieving long molecular dynamics simulation times. ParSplice parallelizes time, allowing effective use of massively parallel computers, and it can be made arbitrarily accurate. We demonstrated ParSplice on the Laboratory's Trinity supercomputer, applying it to a number of challenging applications, including fusion energy materials, diffusion in complex oxides, and evolution of metallic nanoparticles. ParSplice is now the core of a DOE-funded Exascale Computing Project (ECP) effort.

Publications

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Globally Optimal Sparse Representations

Brendt Wohlberg
20150467ER

Project Description

The work is primarily mathematical and computation, consisting of the development of relevant mathematical theory and algorithms, and efficient implementation of these algorithms. The major technical goals are the development of theory, algorithms, and applications of the globally optimal sparse representations. We will develop signal processing theory and methods, together with associated algorithms. If successful, these developments have the potential to change the standard practice in the application of sparse representation methods to a wide variety of problems, together with improved performance and new capabilities of these methods. Specific potential application areas that have already been identified include analysis of radio frequency data for non-proliferation monitoring, analysis of remote sensing data for non-proliferation and intelligence acquisition, modeling of material properties and analysis of multiple modalities of materials science, structural health monitoring for machinery, and analysis of astronomical and sky-survey data.

Technical Outcomes

The technical outcome of this project was the development of efficient algorithms and signal processing techniques for exploiting "convolutional sparse representations" (a new form of a well-established and very effective data modeling technique) for signal and image processing problems. State-of-the-art algorithms were developed both for learning and applying these models; specific applications that were addressed include audio signal analysis, image denoising and deconvolution, and anomaly detection problems.

Publications

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Inserting Nonlinear N-Material Coupling PDF Information into Turbulent Mixing Models

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20150498ER

Project Description

The work develops and implements new mathematical models for multi-component turbulent flows involving materials with very different properties by inserting high-order constrained statistical information into low-order turbulent mixing models. The new turbulent material mix model will correctly account for the nonlinear coupling and constrained statistics in the mixing of multiple materials that do not exist in current approaches and will avoid the conventional/inadequate passive-scalar approximations. The new model will be implemented in a production code for immediate impact on programmatic efforts. We expect sizable improvements over the currently used passive-scalar approximations for multi-material mixing problems. This work will directly and immediately impact modeling efforts and also advance the predictive science in ASC and several science campaigns. The work will result in engineering models, directly relevant to Los Alamos' large physics codes, in which the resolution of all scales are intractable and statistical methods are the only practical approach.

Technical Outcomes

We have developed and validated a new engineering (statistical) model for the small-scale mixing of two very different materials (e.g., gaseous Hydrogen and Iron) in turbulent flows, for the first time correctly capturing the full time-evolution of the highly non-equilibrium physical process of a Rayleigh-Taylor flow, starting from quiescent state, transitioning to laminar then turbulent flow, and dissipative decay. The new model is directly applicable and will be implemented into the Laboratory's hydrodynamics codes.

Publications

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Enabling Automatic Parallelism and Transparent Fault Tolerance

Marion Davis
20150485ER

Project Description

This project entails the design, implementation, and evaluation of a computer programming system that enables high performance and automatic parallelism under various evaluation strategies. High performance computing is fundamental to the advancement of many areas of science. While innovations in hardware technologies continue to allow us to build ever more powerful and complex computing systems, our modes of programming them have advanced conservatively. We are faced with the need to re-examine the entire software stack that ranges from operating systems, runtime systems, programming systems, and applications. At the level of programming systems, the need to re-explore functional language concepts has been explicitly identified. This project directly addresses this need, as well as its corresponding runtime system. Breakthroughs in this area will benefit high performance scientific computing at large, and all scientific disciplines that use it.

Technical Outcomes

We have demonstrated the first open-source, compiled, strict-by-default, higher-order, polymorphic, strongly-typed pure functional computer-programming language implementation. Additional developments include the first higher-order, polymorphic demand analysis capable of inferring degrees of data-structure strictness and a formal extension to an extant framework for generalized Hindley-Milner type inference.

Publications

Davis, K., D. Prichard, D. Ringo, L. Anderson, and J. Marks.
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Presented at *Trends in Functional Programming*. (College Park, Maryland, 8-10 June 2016).

Cyberphysical Systems and Security

Scott Backhaus
20150215DR

Project Description

This project will develop algorithms for detecting, localizing, and defending against attackers in cyberphysical systems, such as electrical grid control systems. Intrusion detection and localization are crucial to the defense of cyber-physical systems but they alone are not sufficient. If a system is under attack, it cannot simply be brought down to purge the attacker; doing so would grant the attacker his objectives, i.e. widespread denial of the services from the cyber-physical network. This work will develop advanced approaches to cyber-physical defense, broken down into the following goals: 1) Detect and localize an attacker within the cyber-physical network without reference to a predefined attack vector; 2) Develop algorithms for proportional response and design resilient cyber-physical networks; 3) Deploy, demonstrate, and validate.

<http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=7836681&isnumber=7836631>.

Technical Outcomes

We developed model-free algorithms to detect intrusions into cyberphysical systems using physical sensor data, communications data and combinations of the data sources. These algorithms were developed on a comprehensive data base of cyberphysical data acquired from a real-world building automation system (BAS), including labelled, ground-truth attack on the BAS. The model-free approach in this project enables rapid transferability of algorithms between cyberphysical systems to avoid high first-costs of modeling building.

Publications

Plasse, J., J. Noble, and K. Myers. An adaptive modeling framework for bivariate data Streams with applications to change detection in cyber-physical systems. To appear in *2017 Data Mining for Cyberphysical and Industrial Systems* .(New Orleans, LA, Nov 18, 2017).

Lokhov, A. Y., N. Lemons, T. C. McAndrew, A. Hagberg, and S. Backhaus. Detection of faults and intrusions in cyber-physical systems from physical correlations. 2016. *2016 IEEE 16th International Conference on Data Mining Workshops (ICDMW)*. 303-310.

Scalable Codesign Performance Prediction for Computational Physics

Stephan Eidenbenz
20150098DR

Project Description

We will develop a performance-prediction capability that relies on modeling architectural and algorithmic details of a computational-physics code running on a specified high-performance computing (HPC) architecture. Based on results for different application domains and on preliminary analysis for transport and hydrodynamics, we anticipate achieving at least one order of magnitude performance improvement for stochastic radiation transport codes as these codes have undergone few optimization efforts for current node designs of many cores and more complicated memory hierarchies. Our future computational physics code base for hydrodynamics and radiation transport are of fundamental importance to DOE and the Laboratory.

Technical Outcomes

This project developed the Performance Prediction Toolkit (PPT): a collection of hardware architecture models, middleware models, and computational physics application models that mimic the execution of computer software on computer hardware using parallel discrete event simulation as the modeling tool. The project open-sourced the underlying Simian simulation engine in the first year of the project and is almost complete with the process of open-sourcing the rest of PPT.

Publications

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Detecting Events Through Graph-Mediated Sensor Consensus

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20170659ER

Project Description

Is something about to happen? Is something happening? Did something just happen? These are the core questions that cut across many sentinel application areas such as nuclear detonation detection, counterterrorism, cyber security, and epidemiology. Multi-sensor networks have generated large quantities of data; however, knowledge discovery has lagged behind, particularly when processes of interest are characterized by multiple, disparate, inconclusive signals. This project resulted in an innovative method for the discovery of an active process of concern. Our work captured the relational and time-scale aspects of events transpiring in time and provides a framework to answer a key question in sensor integration, namely whether an event of interest is underway. Furthermore, it enables direct modeling and incorporation of subject matter expertise in events and processes to build an algorithmic capability for detection and characterization of events in real time. Finally, this project developed novel methods for dynamic cognitive situational awareness in sentinel and early warning systems. This is applicable to a wide variety of specific DOE/NNSA tasks in monitoring for nuclear safeguards and non-proliferation, counterterrorism, and infectious disease outbreak early warning and monitoring. It also has applicability to the DoD mission space with strategic communication in denied environments and electronic warfare.

Technical Outcomes

This project realized an innovative algorithmic framework that enables synergistic relational and multiscale analysis of sensor data and allows explicit incorporation of Subject Matter Expert (SME) process knowledge via forward model template graphs. This was the project's key contribution and innovation. Computer algorithms and software for multiscale analysis of graph time series were developed and applied to real data -the LANSCE accelerator beam operations dataset. Twelve sensors were isolated as showing group anomalous behavior.

Publications

- Prasad, L. Multiscale graph-based framework for efficient multi-sensor integration and event detection. Presented at *SPIE Defense+Security Symposium*.(Orlando, 15-19 Apr. 2018).
- Ferson, S., and K. Sentz. Dependence among probability boxes in fault trees. Presented at *17th International Conference on Information Processing and Management of Uncertainty (IPMU) in Knowledge-Based Systems*.(Cadiz, Spain, 11-15 Jun. 2018).
- Ferson, S., and K. Sentz. Dependence in boolean expressions (poster). Presented at *International Symposium on Imprecise Probabilities and Their Applications (ISIPTA)*. (gano, Switzerland, 10-14 Jul. 2017).

Quantifying the Value of Real-time Social Internet Data for Diverse Forecasting of Dynamic Phenomena: Feasibility study

Sara Del Valle
20160658ER

Project Description

This project will develop a capability to characterize the potential threat of violent extremism with quantified uncertainty. In addition, it will fill in key gaps in developing the scientific foundation for coupling big data and models to inform policy. The anticipated result of the work is a proof-of-concept showing the potential applicability of Internet data streams and social network approaches to monitor emerging threats such as violent acts. This project will enable real-time forecasting of dynamic phenomena informed by multiple, heterogeneous data streams by leveraging the team's success in disease forecasting. The resulting scientific advances and situational awareness will advance our nation's ability to understand, detect, and address multiple threats by leveraging Internet data.

Technical Outcomes

Predicting low frequency events is an important problem with national security implications. We analyzed 33 school shooting incidents from 2010 to 2017. The results show that the summer is the only important covariate and that Twitter chatter does not play a role in predicting future events. There is a 5% chance of a school shooting occurring in the summer and a 10% chance during non-summer months. It is nearly impossible to predict school shootings.

Secure Compositional Computation

Boris Gelfand
20170681ER

Project Description

This project set out to develop new techniques to create “computation” out of observed complex interactions of naturally-occurring components (e.g. biological) or digital-physical systems designed without computation in mind. This research is anticipated to have tremendous benefits in secure computing, authentication mechanisms, and data storage in future cyber-physical systems. Initial applications are most suited to national defense and energy applications and could create a basis for broader application in the computing industry.

Technical Outcomes

We have identified two pools of DNA randomness in the human immune system that provide the necessary biological key material for modern cryptography at the human-machine interface. The pools of randomness are the failed DNA recombinations found in immune T-cell and B-cell populations. These pools of randomness can be queried (read), and are invisible to non-intrusive DNA sampling methods (private). T-cells have 20-40 bits of randomness, B-cells approximately 70 bits, both resist easy phenotypic determination.

Rapid Response: Using LANL's DWave Quantum Computer

Stephan Eidenbenz
20170616ER

Project Description

The goal of this project is to study the possibilities and limitations that the new technology of quantum annealing holds with respect to its scaling. The project will have efforts along the lines of the main use cases of quantum annealers: (1) combinatorial optimization, (2) machine Learning, (3) understanding the physical processes active in the machine and (4) middleware, as well as novel use cases.

Technical Outcomes

Five topics were pursued in the context of quantum annealing on the Laboratory's DWave Quantum Annealer "Ising". *Problem Reformulation and Matrix Sparsification *Graph Partitioning for Electronic Structure Problems *Nonnegative/Binary Matrix Factorization with a D-Wave Quantum Annealer *Rigorous Comparison of the DWave to Established B-QP Solution Methods *Solving Sparse Representation as for Object Classification Using the D-Wave 2X Research resulted in determination of and improvements in machine scalability though algorithmic design, where possible.

Publications

T. Nguyen, Nga T., Amy E. Larson, and Garret T. Kenyon.

Generating sparse representations using quantum annealing Comparison to classical algorithms. To appear in *proceedings of the IEEE International Conference on Rebooting Computing, IRC 2017*.(Washington, DC, USA , November 8-9th, 2017).

Chapuis, G., H. Djidjev, G. Hahn, and G. Rizk. Finding Maximum Cliques on a Quantum Annealer. 2017. In *Proceedings of the Computing Frontiers Conference*.p. 63. <http://doi.acm.org/10.1145/3075564.3075575>.

Coffrin, C., H. Nagarajan , and R. Bent. Ising Processing units: potential and challenges for discrete optimization. 2017. *arXiv:1707.0035*.

Djidjev, H., G. Chapuis , and G. Rizk. Finding Maximum Cliques Using Quantum Annealing. To appear in *ACM International*

Conference on Computing Frontiers.(Siena, Italy, May 15-17th, 2017).

Mniszewski, M., H. Ushijima-Mwesigwa, and C. F. A. Negre. Graph Partitioning using the D-Wave for electronic Structure Problems . To appear in *2017 SIAM Annual Meeting, Minisymposium MS43: Identifying Computational Methods for early Benefit from Quantum Computing*.(Pittsburgh, Pennsylvania, USA, July 10-14, 2017).

Hahn, G., and H. Djidjev. Reducing Binary Quadratic Forms for More Scalable Quantum Annealing. To appear in *IEEE International Conference on Rebooting Computing*. (Washington, DC , November 8-9, 2017).

Hahn, G., H. Djidjev, and G. Rizk . Efficient Combinatorial Optimization for Graph Partitioning Using Quantum Annealing. To appear in *SIAM Conference on Optimization*. (Vancouver, British Columbia, Canada, May 22-25, 2017).

and Velimir V. Vess, Daniel O'Malley Nonnegative/binary matrix factorization with a D-Wave quantum annealer. 2017. *CoRR*. **abs/1704.01605**. <http://arxiv.org/abs/1704.01605>.

Ushijima-Mwesigwa, H., C.F. A. Negre, and S. M. Mniszewski. Graph Partitioning using Quantum Annealing on the D-Wave system. To appear in *ACM SC 2017 PMES*.(Denver, Colorado, November 13, 2017).

Process Tree Signature Detection

Peter Hraber
20170682ER

Project Description

Cybersecurity needs new methods to detect malicious software in real-time, not retroactively. Antivirus signatures aim to do this but are defeated by new exploits and obfuscation. Signatures of pathological or misbehaving processes could enable rapid incident detection and response. Computer operating systems are hierarchical: an initial root process creates many child processes, which in turn start and run descendants. Creation and termination of new processes are logged by a computer's accounting services, centrally recorded and archived. This data resource is a learning opportunity. This project developed methods to infer process hierarchies and compare their properties, using data from over 10,000 Los Alamos National Laboratory Windows computers. Properties of interest include what type of children a process creates, how frequently it creates them, and whether a human user or the operating system initiated it. A new collaboration formed between Los Alamos cybersecurity experts and a computational biologist with expertise in viral genomics, which includes methods to model within-host evolution and to infer, compare, and manipulate trees. The project supported multidisciplinary research to grow new capabilities, and made innovative use of unique Los Alamos resources. Process hierarchies remain an underexplored topic in cybersecurity research, with strong potential for real-time cybersecurity event detection.

models and labeled data are still needed to define anomalous events and enable rapid incident detection.

Technical Outcomes

Computer systems operate hierarchically. The root process starts other processes, which start descendants. Process creation is centrally logged, recorded, and archived. Using this data resource, we characterize the range of behaviors seen on an enterprise-scale network. We inferred process hierarchies from Windows-logging system process-creation events, evaluated alternative criteria to define such hierarchies, and compared hierarchies between hosts. Calibrated probabilistic

Automated Design of Network Security Metrics using Self-Adaptive Hyper-Heuristics

Aaron Pope
20170683ER

Project Description

In an age where new software vulnerabilities are discovered and exploited on a daily basis, best practices and expedient response are not enough to secure a large computer network. Administrators need to be able to understand, analyze, and track the level of security in networks they manage. As enterprise computer networks continue to grow in size and complexity, manual methods of analyzing network security are often insufficient. Automated analysis tools are needed to highlight vulnerabilities and allow a pro-active defense strategy. This work demonstrates the application of a novel machine learning technique to automate the development of network security metrics. The approach is tested and verified using a simulation based on Los Alamos network activity. This work contributes to the field of automated heuristic design and optimization. Additionally, this work provides a new capability to rapidly evolve and react to emerging cybersecurity threats.

Technical Outcomes

This work demonstrated the application of a novel self-adaptive hyper-heuristic machine learning technique to automate the development of network security metrics. The approach was tested and verified using a simulation based on Los Alamos National Laboratory network activity. This work contributes to the field of automated heuristic design and optimization. Additionally, this work provides a new capability to rapidly evolve and react to emerging cybersecurity threats.

Deep Sparse Columnar Neural Network (dSCANN)

Garrett Kenyon
20150752ER

Project Description

We aim to demonstrate how a scalable cortical architecture can learn to use visual cues to represent depth within a scene in an entirely unsupervised manner, analogous to how biological systems are hypothesized to self-organize during visual development. Deep-learning algorithms based on convolutional neural networks loosely inspired by brain architecture have become the state of the art for classes of problems such as object/image classification and pattern recognition. These are problems that have not been adequately addressed with conventional algorithms. Using the Los Alamos supercomputer Trinity, we will implement a novel neural network architecture based on the columnar organization of the cerebral cortex. The results of this work could result in new methods for automating the analysis of large data streams using supercomputer resources, and advance the state-of-the-art in automated spatial navigation and target detection tasks.

Competitive Algorithm for Building Sparse Hierarchical Representations. 2016. In *Computational Models of the Visual Cortex, 9th EAI International Conference on Bio-inspired Information and Communications Technologies*. (Columbia University, New York, 2015). p. 0. New York: EUDL. <http://eudl.eu/doi/10.4108/eai.3-12-2015.2262428>.

Technical Outcomes

We implemented a new type of deep neural network called a sparse prediction machine on the Trinity supercomputer at the Los Alamos National Laboratory. Our software exhibited efficient scaling across thousands of Intel Knights Landing processors. Our results demonstrated that we could learn to predict future video frames from previous frames and suggest a strategy for using neural networks to accelerate large scale physical simulations on future instantiations of ultra low power neuromorphic hardware.

Publications

Lundquist, S. Y., D. M. Paiton, P. Schultz, and G. T. Kenyon. Sparse Encoding of Binocular Images for Depth Inference. 2016. In *2016 IEEE Southwest Symposium on Image Analysis and Interpretation*. (Santa Fe, 6-8 March, 2016). Vol. 0, 0 Edition, p. 121. Santa Fe: IEEE. <http://https://goo.gl/FQieqH>.

Paiton, D. M., X. Zhang, S. Y. Lundquist, W. Shainin, P. Schultz, and G. T. Kenyon. A Deconvolutional



Materials for the Future

Target Projects in Theoretical and Experimental Materials Science: Novel Structural Models, Materials Imaging and Informatics, and Strength/Sensing Capabilities Integrated During Manufacturing.

Alexander Balatsky
20160651ER

Project Description

We focus on developing new materials and design principles to enable better performance of batteries, computer memory, solar devices, and ultra light weight armor. Goals we aim to accomplish include: utilize adaptive feedback for faster 3D measurements of mesoscale materials; develop the computation capabilities to predict layered materials with emergent properties; develop methodologies to create 3D-printed fuel cell electrodes; develop techniques to create lighter than air solids; and develop novel memristors at vertical nanointerfaces with ultrahigh storage density.

Publications

- Julien, J. P., J. D. Kress, and J. X. Zhu. Explicit inclusion of electronic correlation effects in molecular dynamics. 2017. *Physical Reviews B*. **96**: 035111.
- S. Rosa, P. F., S. M. Thomas, F. F. Balakirev, J. Betts, S. Seo, E. D. Bauer, J. D. Thompson, and M. Jaime. An FBG optical approach to thermal expansion measurements under hydrostatic pressure. 2017. *Sensors*. **17**: S17112543.
- Ronning, F., T. Helm, K. R. Shirer, M. D. Bachmann, I. Balicas, M. K. Chan, B. J. Ramshaw, R. D. McDonald, F. F. Balakirev, M. Jaime, E. D. Bauer, and P. J. W. Moll. Electronic in-plane symmetry breaking at field-tuned quantum criticality in CeRhIn5. 2017. *Nature*. **548**: 313.
- Cherukara, M. J., R. Pokharel, T. S. OLeary, J. K. Baldwin, E. Maxey, W. Cha, J. Maser, R. J. Harder, S. J. Fensin, and R. L. Sandberg. Three-dimensional X-ray diffraction imaging of dislocations in polycrystalline metals under tensile loading . Submitted to *Nature Communications* .
- Jaime, M., C. C. Moya, F. Weickert, V. Zapf, F. F. Balakirev, M. Wartenbe, P. F. S. Rosa, J. B. Betts, G. Rodriguez, S. A. Crooker, and R. Daou. Fiber bragg grating dilatometry in extreme magnetic field and cryogenic conditions. 2017. *Sensors*. **17**: s17112572.

Investigating Complex Superconducting Phases via Field-Rotating Transport and Thermodynamic Measurements

Roman Movshovich
20150762PRD4

Project Description

We will conduct thermal conductivity and specific measurements in a high magnetic field (14 Tesla) and a very low temperature (down to 20 milliKelvins) to probe the nature of unconventional superconducting states. This project will address the issue of unconventional superconductivity, by directly measuring the symmetry of the superconducting order parameter in a number of compounds. Some states that will be explored represent unique states of matter. This research is therefore of great interest to the mission of the basic understanding of materials.

Publications

Kim, D. Y., Lin, Weickert, Kenzelmann, E. D. Bauer, Ronning, J. D. Thompson, and Movshovich. Intertwined Orders in Heavy-Fermion Superconductor CeCoIn₅. 2016. *PHYSICAL REVIEW X*. **6** (4).

Kim, D. Y., Lin, E. D. Bauer, Ronning, J. D. Thompson, and Movshovich. Switching dynamics of the spin density wave in superconducting CeCoIn₅. 2017. *PHYSICAL REVIEW B*. **95** (24).

Kim, D. Y., Lin, Weickert, E. D. Bauer, Ronning, J. D. Thompson, and Movshovich. Resonances in the Field-Angle-Resolved Thermal Conductivity of CeCoIn₅. 2017. *PHYSICAL REVIEW LETTERS*. **118** (19).

Chemical Vapor Growth of Hybrid-Perovskite Materials for Next-Generation Energy

Aditya Mohite
20160680PRD4

Project Description

Chemical vapor deposition (CVD) of hybrid perovskites is expected to be transformational, enabling the growth of highly crystalline, reproducible, and stable materials that could accelerate the implementation of perovskite-based materials for a broad range of energy and optoelectronic applications. CVD grown hybrid-perovskite materials for next-generation energy is going to contribute to the national economy through development of important new environmental strategy to design and develop new perovskites materials for optoelectronic applications, and pave the way for the development of novel materials to the overall our Nation's energy security.

Understanding Non-Collinear Magnets: From Crystal Structure to Magnetic Function

Eric Bauer
20160679PRD4

Project Description

The project proposes to discover new, unusual non-collinear/non-coplanar magnets to understand how structure controls magnetic functionality. These magnets are promising candidates for future memory storage devices or as sensors. The discovery and understanding of novel topological and unconventional superconducting states is at the forefront of condensed matter research. Finding a new superconducting helimagnet, a novel spin structure, a large Hall effect, or other unusual temperature dependent of the physical properties in a non-collinear magnet would be a significant advance because it would uncover the mechanism required to generate these novel states of matter. This project will provide insight into unusual spin structures, which could be used as the basis for future electronics applications.

Publications

Sung, N. H., F. Ronning, J. D. Thompson, and E. D. Bauer.
Magnetic Phase Dependence of the Anomalous Hall Effect
in Mn₃Sn single crystals. Submitted to *Physical Review B*.

In Situ Quantification and Characterization of Phase Evolution during Metal Additive Manufacturing

John Carpenter
20170641ER

Project Description

Using a Los Alamos built experimental rig, additive manufacturing will be conducted in a high energy beamline with the x-rays providing diffraction data that will help us understand how the metal is cooling and solidifying. The time and length scales we will be achieving experimentally are significant improvements over earlier experiments and will exploit the cutting edge available in detectors and diagnostics to achieve these improvements. The data obtained will both motivate and inform microstructural evolution models which do not currently exist because of the dearth of experimental data at the correct time and length scales. With these models in hand, we could potentially exploit the additive manufacturing process to create materials with microstructures that exhibit enhanced properties and performance. In addition, this information is critical for understanding the science behind using additive manufacturing as a repair or refurbishment technology for components important to programmatic missions within the NNSA.

Thompson. In situ neutron diffraction measurements during uniaxial loading of additively manufactured GP1 stainless steel. 2017. *Materials Science and Engineering A*. **696**: 331-340.

Publications

Stockman, T., J. A. Schneider, C. M. Knapp, and J. S. Carpenter. Defect detection in LENS AM using in situ thermal camera process monitoring. To appear in *2018 TMS Annual Meeting*. (Phoenix, 11-15 March 2018).

Pokharel, R., V. Livescu, D. W. Brown, B. Clausen, J. S. Carpenter, G. T. Gray, S. C. Vogel, C. M. Knapp, and D. P. Adams. Influence of additive manufacturing techniques on mechanical properties and microstructures of 304L stainless steel. Submitted to *Acta Materialia*.

Brown, D. W., D. P. Adams, L. Balogh, J. S. Carpenter, B. Clausen, G. M. King, B. Reedlunn, T. A. Palmer, M. C. Maguire, and S. C. Vogel. In situ neutron diffraction study of the influence of microstructure on the mechanical response of additively manufactured 304L stainless steel. To appear in *Metallurgical and Materials Transactions A*.

Clausen, B., D. W. Brown, J. S. Carpenter, K. D. Clarke, A. J. Clarke, S. C. Vogel, J. D. Bernardin, D. Spornjak, and J. M.

Formation, Stability, and Chemistry of Tetravalent Actinide Nanocrystals

Ping Yang
20160604ECR

Project Description

This project directly addresses a widely known scientific problem of understanding the fundamental bonding interactions involved with 5f-electrons in order to master the chemistry and physics of actinides and actinide-bearing materials. 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.

Publications

Wang, G., E. R. Batista, and P. Yang. Ligands induced shape transformation of thorium dioxide nanocrystals. Submitted to *ACS Nano*.

Plasmonics-Transformed Quantum Emitters Through Theory-Guided Synthesis

Jennifer Hollingsworth
20160653PRD2

Project Description

We will transform quantum emitters through plasmonics to be ideal single- and entangled-photon-pair sources. The new semiconducting-metallic nanostructures will have unique properties that cannot be obtained in either type of material alone. The work will provide new fundamental understanding for the design of controlled plasmon-photon interactions across scale, which will underpin the advancement of quantum dots as gain media for cavity-enhanced lasers. Such advanced light emitters are needed for next-gen communications and computing (light-enabled or even all-optical networks).

Hu, Z., A. Singh, S. Goupalov, J. A. Hollingsworth, and H. Htoon. Probing morphological effects on photoluminescence properties in single colloidal nanoplatelets. Submitted to *Nature Communications*.

Publications

Hanson, C. J., N. F. Hartmann, Singh, Ma, W. J. I. DeBenedetti, J. L. Casson, J. K. Grey, Y. J. Chabal, A. V. Malko, Sykora, Piryatinski, H. a. n. Htoon, and J. A. Hollingsworth. Giant PbSe/CdSe/CdSe Quantum Dots: Crystal-Structure-Defined Ultrastable Near-Infrared Photoluminescence from Single Nanocrystals. 2017. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*. **139** (32): 11081-11088.

Orfield, N., S. Majumder, J. McBride, F. Koh, A. Singh, J. Casson, J. Hollingsworth, and H. Htoon. Thermally-Assisted Photobleaching Mechanisms of "Giant" Quantum Dots Revealed in Single Nanocrystals. Submitted to *ACS Nano*.

Peer., Hu, Singh, J. A. Hollingsworth, Biswas, and H. a. n. Htoon. Photoluminescence Enhancement of CuInS₂ Quantum Dots in Solution Coupled to Plasmonic Gold Nanocup Array. 2017. *SMALL*. **13** (33).

Coughlan., Ibanez, Dobrozhan, Singh, Cabot, and K. M. Ryan. Compound Copper Chalcogenide Nanocrystals. 2017. *CHEMICAL REVIEWS*. **117** (9): 5865-6109.

Krishnamurthy, S., A. Singh, Z. Hu, A. Malko, H. Htoon, and J. Hollingsworth. Controlling blinking and device performance using shell thickness in infrared quantum dots. Submitted to *Nature Material*.

Singh, A., S. Majumder, N. J. Orfield, D. Nordlund, K. Bustillo, J. Ciston, H. Htoon, and J. A. Hollingsworth. From inside out: how buried interface, defects and surface determines performance of two giant core/shell quantum dots. Submitted to *SCIENCE*.

Deoxyribonucleic Acid (DNA) Mediated Photonic Superstructures for Enhanced Artificial Photosynthesis

Sergei Ivanov
20160675PRD3

Project Description

This research project directly addresses energy needs of the future, which is a critical national security challenge. A goal within this challenge is to enhance the efficiency of capture and utilization of light (photonic) energy for materials applications, such as improving efficiency in photovoltaics and solid-state lighting. This project seeks to develop molecular-scaled materials, based upon DNA and polymers, which exhibit dynamic photonic properties and can be incorporated to existing photonic platforms for enhanced efficiency through dynamic regulation. Hybrid constructs consisting of DNA-polymer assemblies will be synthesized for this study. The polymer component induces material stability and device integration in a stimuli-responsive matrix, as well as serves as a home for photonic chromophores and the DNA allows for creation of clusters of metal ions that result in tunable light response. Coupled together, these constructs have the potential of exhibiting a wide breadth of tunable photonic response not typically observed in photonic materials. Coupling to existing platforms could result in new classes of tunable, efficient photonic materials for a range of applications.

Materials for the Future

Postdoctoral Research & Development
Continuing Project

A Gruneisen Approach to Quantum Criticality

Priscila Ferrari Silveira Rosa
20170667PRD1

Project Description

An important aspect of the 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.

Toward Controlled Synthesis of Actinide Oxide Nanocrystals: A Theoretical Perspective

Enrique Batista
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.

Publications

Wang, G., p. Yang, N. A. Moody, and E. R. Batista. Atomically thin two dimensional materials for photocathodes protection: Engineering the work function through induced interface dipoles . Submitted to *Nature Communication*.

Wang, G., E. R. Batista, and P. Yang. Ligands induced shape transformation of thorium dioxide nanocrystals . Submitted to *ACS Nano*.

Macroporous/Nanoporous Hierarchical Carbon Structure (MNHCS) for High-Performance Energy Storage Devices

Jeffrey Pietryga
20150760PRD4

Project Description

This project aims to develop next-generation, carbon-based porous materials for high performance energy storage devices such as lithium ion batteries and supercapacitors. We expect to achieve synthesis of 3D reduced nanoporous graphene oxides and fullerene-based composites that offer several unique properties: i) an interconnected electrolyte-filled macroporous network that enables increased contact surfaces between the 3D network and electrolytic solution, and rapid ion transport, ii) short ion and electron transport lengths, iii) a high electrode specific surface area and (iv) high electron conductivity in the electrode assembly. This method will be extended to the synthesis of a variety of 3D conjugated systems that will render the formation of conducting macroporous/nanoporous structures, ideally suited for the fabrication of highly efficient supercapacitors and lithium ion batteries. Success in this project will have widespread impact on the development of high performance energy storage technologies.

Publications

Shan, J., Yen, Wu, Lin, Zhou, Guo, D. i. Wu, Zhang, Wu, and Wang. Functionalized fullerenes for highly efficient lithium ion storage: Structure-property-performance correlation with energy implications. 2017. *NANO ENERGY*. **40**: 327-335.

Shan, C., K. Wu, H. J. Yen, C. N. Villarrubia, T. Nakotte, X. Bo, G. Wu, and H. L. Wang. Graphene oxides used as a new “dual role” binder for stabilizing silicon nanoparticles in lithium ion battery. Submitted to *ACS Applied Materials and Interfaces*.

Connecting Interface Structure and Functionality in Oxide Composites

Blas Uberuaga
20160501ER

Project Description

Using atomistic and mesoscale modeling, combined with experimental synthesis and characterization, we will determine the relationship between interfacial atomic structure and ionic conductivity in complex oxide heterostructures. Many technologically important applications, ranging from solid-oxide fuel cells, to supercapacitors, rely on materials that exhibit high ionic conductivity -- these are referred to as superionic. Despite the promise of these materials and the intensive research accompanying them, they still fall short of expectations. Not only will our work enable improved materials for applications such as fuel cells and supercapacitors, it will also enable control of mass transport in complex materials via interfacial properties. This will be a first for Los Alamos, leading to a new ability to design materials for advanced applications involving superionics.

Publications

Dholabhai, P. P., Martinez, N. T. Brown, and B. P. Uberuaga.
On the mobility of carriers at semi-coherent oxide heterointerfaces. 2017. *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. **19** (34): 23122-23130.

Controlling the Functionality of Materials through Interfacial Colloidal Gelation

Matthew Lee
20160519ER

Project Description

We will develop new synthetic routes for high-performance materials utilizing nano-scale particles as building blocks for complex structures vital to many modern technologies, including catalytic and energy systems (e.g. batteries). The project goal is a rational design of porous and composite solids with controlled interfacial functionality using an emerging class of soft matter known as bicontinuous interfacially jammed emulsion gels, or Bijels. Because Bijels are a recent invention, our fundamental understandings of their physical assembly, aging, and mechanical properties are at an early stage. Moreover, Bijels have vast untapped potential in an array of current engineering applications, including interfacial catalysis and renewable energy systems. Successful realization of the proposed research objectives will provide critical advances in both theoretical modeling of multi-phase soft materials and novel materials synthesis techniques, paving the way for new generations of functional porous and composite solids for a diverse array of applications, including optimized energy storage devices and waste management and remediation technologies.

Publications

Santiago-Cordoba, M., K. J. Cluff, C. E. Hamilton, C. Grote, E. Weis, M. Herman, N. Parra-Vasquez, and M. N. Lee. Accelerating the Design of Low Density Materials with Bicontinuous and Hierarchical Porosity for Enhanced Energy-Driven Applications . 2016. In *Materials Research Society Fall 2016 Meeting & Exhibition*.(Boston, Nov. 27th - Dec. 2nd 2016). p. 0. Boston: Materials Research Society.

Welch, P. M., M. N. Lee, A. N. G. Parra-Vasquez, and C. F. Welch. Jammed Limit of Bijel Structure Formation. To appear in *Langmuir*.

Exotic States in U-based Superconductors

Roman Movshovich
20160572ER

Project Description

This project aims to determine the symmetry of the superconducting order parameter in a number of uranium-based superconductors with different magnetically ordered ground states, and correlate that symmetry with the nature of those related magnetic state. Uranium-based heavy fermion compounds offer a particularly fertile area to look for an emergent behavior, as they present a large variety of magnetically ordered ground states that seem to be connected to superconductivity. We will correlate the order parameter symmetry with the nature of magnetic fluctuations, accessing the microscopic origins of superconductivity in selected U-based superconductors. These results will help understand the origins of unconventional superconductivity in a wider range of materials, including high temperature cuprate and pnictide superconductors.

Publications

Kim, D. Y., Lin, E. D. Bauer, Ronning, J. D. Thompson, and Movshovich. Switching dynamics of the spin density wave in superconducting CeCoIn₅. 2017. *PHYSICAL REVIEW B*. **95** (24).

Kim, D. Y., Lin, Weickert, E. D. Bauer, Ronning, J. D. Thompson, and Movshovich. Resonances in the Field-Angle-Resolved Thermal Conductivity of CeCoIn₅. 2017. *PHYSICAL REVIEW LETTERS*. **118** (19).

Kim, D. Y., Lin, Weickert, Kenzelmann, E. D. Bauer, Ronning, J. D. Thompson, and Movshovich. Intertwined Orders in Heavy-Fermion Superconductor CeCoIn₅. 2016. *PHYSICAL REVIEW X*. **6** (4).

Quantum Optics of Solitary Covalent Dopants in Carbon Nanotubes

Han Htoon
20160172ER

Project Description

With this project, we aim to establish doped carbon nanotubes that can be synthesized at a very low cost as a new transformational material for making light sources that emit one photon at a time (single photon sources) and switches that could control a stream of single photons: two fundamental building blocks needed for the realization of eavesdropping proof quantum communication technology. In addition, single photon sources can also enable quantum meteorology technology, in which absorption of the light can be measured beyond the shot-noise limit of typical laser light sources. Such technology could enable novel ultra-sensitive sensing platforms. Results of this project could help protect information critical for national security. The work directly addresses information collection, surveillance and reconnaissance, and national defense missions.

Publications

Htoon, H. New Building Blocks for Quantum Technologies: Doped Carbon Nanotubes and Plasmonically Coupled Quantum Dots Molecules . Presented at *META'16, the 7th International Conference on Metamaterials, Photonic Crystals and Plasmonics*.(Melag, Spain, 25-28 July, 2016).

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Nonequilibrium Dynamics and Controlled Transport in Skyrmion Lattices in Nanostructures

Charles Reichhardt
20160369ER

Project Description

We aim to understand how a very small magnetic object called a skyrmion can be dynamically controlled. Skyrmions could act as smaller, more robust, more energy-efficient information carriers for computers. We will model and understand how to precisely control skyrmion motion in nanostructured geometries for the most effective way to move, write, read, and pack skyrmions in dense patterns that remain stable for long times. We will use a combination of continuum and particle-based simulations to model these geometries and driving protocols. The potential to create low-power, high-density magnetic storage devices and other magnetic-based logic devices would have a wide range of applications relevant for national security, including making smaller, more compact, lighter, and less energy costly devices for use by soldiers, aerial vehicles, and drones.

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Emergent and Adaptive Polymers

Jennifer Martinez
20160528ER

Project Description

This project aims to provide multifunctional materials for next-generation polymer light-emitting electrochemical cells (PLECs) and organic light-emitting diodes (OLEDs) used in implantable and wearable electronics. We will create libraries of genetically encoded and optically active polymers, and through a technique akin to evolution, sort for those polymers that exhibit a defined optical or adaptive response. Use of genetically encoded polymers (GEPs) allows us to create large libraries of stimuli-responsive polymers (far eclipsing current synthetic techniques) and to identify, en masse, those polymers with a defined function or physical property in a matter of days instead of decades.

Publications

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Topology and Strong Correlations: A New Paradigm

Filip Ronning
20160085DR

Project Description

This project proposes to identify new materials and new functionalities as a consequence of combining the concepts of topology and electron correlations. We will develop a "materials by design" approach using state-of-the-art theory combined with new and existing experimental capabilities to rapidly identify correlated topological materials with new functionalities. We will explore f-electron based insulators - a natural choice due to their inherent strong electronic correlations and large spin-orbit coupling, which will lead to new topological orders. Our success will lay the foundation for the discovery of new states of correlated topological matter and control over the protected conducting surface states, which are promising candidates for future technologies. With high tenability, reduced dimensionality and large mobilities, these materials can address national security needs in many impact areas including: sensing, metrology, quantum information, nuclear fuels, and spintronics.

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Predicting High Temperature Dislocation Physics in HCP Crystal Structures

Abigail Hunter
20160156ER

Project Description

The primary goals of this project are to use a novel mesoscale model framework to investigate high temperature deformation mechanisms, and predict their effect on the mechanical response of hexagonal close packed metals during manufacturing processes. We will advance a 3D mesoscale code unique to Los Alamos called phase field dislocation dynamics (PFDD). The model aims to bridge the atomic to meso-scale gap, and produce predictive multiscale simulations crucial for understanding dislocation structure evolution under extreme conditions. Continuum-scale material models used in weapons codes lack physically based descriptions of mechanisms that many atomic, nano, and microscale models have shown to be important. The information gained during this project will be used to develop physically based constitutive models to describe strength and damage.

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The influence of anisotropy on the core structure of Shockley partial dislocations with in fcc materials. To appear in *Modelling and Simulation in Materials Science and Engineering*.

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Beyerlein, I. J., and A. Hunter. Understanding dislocation mechanics at the mesoscale using phase field dislocation

Additive Manufacturing of Mesoscale Energetic Materials: Tailoring Explosive Response through Controlled 3D Microstructure.

Alexander Mueller
20160103DR

Project Description

High explosive (HE) structures will be produced via 3D printing techniques to enable studies on detonation science. The understanding gained and capabilities developed by this work will provide the ability to tailor HE performance through structure. This effort will lay the groundwork necessary to fabricate additive manufacturing-HE with novel controlled initiation and reaction zone characteristics by attaining prompt reactive burn through control of the internal structure of the HE part. We aim to tailor shock sensitivity and detonation performance, and envision AM-HE that exhibits better corner-turning capabilities for applications such as more effective HE boosters. Once detonating, the effects of the tailored chemical reaction zone dynamics on detonation critical diameter, confinement edge angles, and failure characteristics will be quantified. A combination of mesoscale-to-continuum scale data will be used to construct a new mesoscale informed reactive burn model.

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Transient Thermal Conduction in Nonlinear Molecular Junctions

Dmitry Yarotski
20160180ER

Project Description

We will apply a unique integration of chemical synthesis, advanced ultrafast optical techniques, and theoretical modeling of nonlinear vibrational dynamics to reveal the mechanisms and test the dynamic limits of thermal transport in DNA molecules. The close communication between the new dynamic thermal probes and theoretical modeling should enable us to resolve the controversy between existing coarse-grained models (that reproduce equilibrium properties of DNA equally well but differ by orders of magnitude in the estimates of the non-equilibrium response) and develop predictive description of complex thermal conductivity of DNA oligomers. The results of this work will strongly impact national security missions that rely on complex systems, nanotechnology and, especially, nanoelectronics, because better understanding of nonlinear heat transfer in molecular-scale systems is an enabling ingredient for technological applications of novel molecular electronic and heattronic/phononic devices.

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Foldamers: Design of Monodisperse Macro-Molecular Structure by Selection of Synthetic Heteropolymer Sequence

Charlie Strauss
20160044DR

Project Description

We propose to design, create, and identify polymers with defined 3D structure and function to provide a new class of materials for catalysis, chem-bio threat reduction, and optical electronics. Control over synthetic polymer 3D architecture ("foldamers") remains a grand challenge in material science. We are creating a fundamentally new class of engineered material with inherently broad impact across many application domains. This is seen by analogy to the bio-materials, proteins, whose unique folding ability enable materials with extreme performance. Our new class of folding material will have similar capabilities but will withstand harsh environmental conditions and can incorporate non-biological dynamic functional materials. This work impacts energy security objectives by establishing novel catalyst materials suited for high-temperature and strong pH in biofuel reactors for the efficient use, generation, storage, and impacts mitigation of energy derived from fossil fuels or renewables entails an energy production/delivery/utilization system. Foldamers can also supply the sophisticated molecular recognition required for hierarchical molecular self-assembly spanning millimeter scales, impacting national advanced manufacturing objectives.

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Frontiers in Quantum Science

Angel Garcia
20160587DR

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 such as skyrmions, and (3) bridge concepts of fluctuation-induced forces with new meta-material technology. This work has relevance in developing new materials for energy applications such as photovoltaic materials, modeling and predicting properties of f-electron matter, including plutonium, for NNSA mission objectives, and developing materials for quantum computing applications.

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Stimuli-Responsive Coordination Polymersomes

Reginaldo Rocha
20160284ER

Project Description

This project aims to create next-generation nanocarriers for controlled transport and triggered release of diagnostic/therapeutic agents in nanomedicine. The proposed systems can also be further applied into emerging self-healing materials technologies. The successful demonstration of functional metallo-polymersomes in this capacity will also have important implications as stimuli-responsive carriers of catalysts and reactants in the realm of electronic, photonic, and energy materials (e.g. damage self-repair and corrosion remediation). Because the broad field encompassing dynamic metallo-supramolecular polymers and functional metal-organic composite materials is still in its infancy, our research undertaking has a great potential for technical leadership and programmatic growth in areas of relevance to Los Alamos missions. There is potential for applications in optically and electronically responsive devices, as well as materials healing and treatment, including nuclear/weapon components.

Publications

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- Elkin, T., J. S. Martinez, G. A. Montano, and R. C. Rocha. Stimuli-Responsive Metallo-Polymers. Presented at *Annual Meeting of the DOE's Center for Integrated Nanotechnologies (CINT)*.(Santa Fe, NM, 25-27 September, 2017).
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Rigorous Development of Atomic Potential Functions in Terms of Strain Functionals

Edward Kober
20160220ER

Project Description

We will develop a robust method for capturing the deformation properties of metals at an atomistic level. The resulting functions will be used in extreme scale simulations of those materials to enable the manufacture of improved materials. The overall goal is to develop atomic potential functions for the molecular dynamics (MD) simulations of metals that capture the very broad range of behavior including mechanical deformation, phase transitions and shock-loading. These will be calibrated to a combination of experimental data and electronic structure calculations. This will enable predictive MD simulations that will accurately capture the behavior of irregular atomic structures found around defects and grain boundaries in metals. This will allow us to more completely understand how the mesoscale structure of a metal affects its response characteristics, and enable the design of improved materials. Understanding the performance properties of metals and developing accurate models that can predict that behavior under a wide variety of circumstances is of critical importance to energy and defense missions, and also of significance to general manufacturing capability.

Publications

Kober, E. M., and S. P. Rudin. Strain functionals for characterizing atomistic geometries and deformation processes. Presented at *American Chemical Society Meeting*.(Philadelphia, 22-25 Aug. 2016).

Mathew, N., S. P. Rudin, and E. M. Kober. Characterizing atomistic geometries and potential functions using strain functionals. Presented at *American Physical Society Meeting*.(St. Louis, 9-14 July 2017).

Kober, E. M., and S. P. Rudin. Strain Functionals for Characterizing Atomistic Geometries and Potential Functions. Presented at *American Physical Society Meeting*.(Baltimore, 15-17 Mar. 2016).

Theory of Spin and Valley Dynamics in 2D Dirac Semiconductors

Nikolai Sinitsyn
20160648PRD2

Project Description

This project will focus on achieving control of spin and valley magnetic moments of electrons in the new class of atomically thin semiconductor materials known as “Dirac semiconductors.” This emerging family of semiconductors is very similar in structure to graphene but superior. The new 2D materials have an optical gap that makes them similar to commercial semiconductor, but being atomically thin and very stable, they will outperform all currently used semiconductors in energy efficiency, solar cells, and quantum information applications. Dirac semiconductors have the potential to replace commercial semiconductors for energy-efficient electronics and solar cell applications.

Publications

- Li, , Sun, V. Y. Chernyak, and N. A. Sinitsyn. Multistate Landau-Zener models with all levels crossing at one point. 2017. *PHYSICAL REVIEW A*. **96** (2).
- Li, , and N. A. Sinitsyn. Dynamic symmetries and quantum nonadiabatic transitions. 2016. *CHEMICAL PHYSICS*. **481**: 28-33.
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- i. Mueller, K. a., Bechtold, Li, Simmet, N. A. Sinitsyn, and J. J. Finley. Optically-probing spin qubit coherence without coherent control. 2017. *ULTRAFAST PHENOMENA AND NANOPHOTONICS XXI*. **10102**.

Microstructural Characterization of Shock-Recovered Explosives for Mesoscale Model Development

John Yeager
20160619ECR

Project Description

We will controllably damage high explosives without detonation, using radiography during the damage event, and recover them afterwards for characterization. This data will be used to improve models that describe damage and detonation of explosives. Relevant fields will be impacted in several ways: 1) soft recovery (i.e. without further damaging the sample) would be a new capability for Los Alamos; 2) this type of mesoscale model has been difficult to validate using real data for high explosives; and 3) long-standing questions about the damage to initiation process will be addressed. Successful execution of this program will provide fundamental understanding of high explosive materials in the form of data and models that inform thermomechanical codes, particularly for abnormal events such as fragment impact or low-pressure shock.

HTPB binder and HMX crystals under tensile loading. To appear in *International Journal of Mechanical Sciences*.

Publications

Walters, D. J., D. J. Luscher, J. D. Yeager, and B. M. Patterson. Investigating deformation and mesoscale void creation in HMX based composites using tomography based grain scale FEM. . To appear in *20th Biennial International Conference of the APS Topical Group on Shock Compression of Condensed Matter (SCCM-2017)*. (St. Louis, 9-14 July 2017).

Manner, V. W., J. D. Yeager, B. M. Patterson, D. J. Walters, J. A. Stull, N. L. Cordes, D. J. Luscher, K. C. Henderson, A. M. Schmalzer, and B. C. Tappan. In Situ Imaging during Compression of Plastic Bonded Explosives for Damage Modeling. 2017. *Materials*. **10** (6): 638.

Yeager, J. D., V. W. Manner, J. A. Stull, D. J. Walters, A. M. Schmalzer, D. J. Luscher, and B. M. Patterson. Importance of microstructural features in mechanical response of cast-cured HMX formulations. To appear in *20th Biennial International Conference of the APS Topical Group on Shock Compression of Condensed Matter (SCCM-2017)*. (St. Louis, 9-14 July 2017).

Walters, D. J., D. J. Luscher, J. D. Yeager, and B. M. Patterson. Cohesive finite element modeling of the delamination of

High Resolution Laser Velocimetry and Ranging for Materials Research

Patrick Younk
20170541ECR

Project Description

With this project, we are developing new technology that will significantly increase the resolution of our laser systems that measure velocity and position in dynamic experiments. This new technology will enhance our capability to perform dynamic experiments relevant to stockpile stewardship and possibly other national security challenges.

Novel Topological Orders in Strongly-Correlated Systems

Jianxin Zhu
20170664PRD1

Project Description

Topology is a branch of mathematics that studies properties that only change incrementally, in integer steps, rather than continuously. For example, for a topologist, the only difference between the three foods --- a cinnamon bun, a bagel, and a pretzel --- is the number of holes in them, rather than their taste. The same idea (characterizing the topology number) can be used to explain phase changes in matter, albeit not familiar ones such as a liquid freezing to a solid or sublimating to gas. The postdoc fellow's work is centered on topological phases of quantum matter. It is aimed to search for novel electronic and spin states that are of huge technological impact. For example, topological insulators block the flow of electrons in their interiors while simultaneously conducting electricity across their surfaces. This unique property could make these quantum materials useful for ferreting out new types of fundamental particles, and for forming circuitry within quantum computers. Scientists are already discussing and in some cases making other even more exotic materials, topological superconductors and topological metals that each hold vast potential for new applications in computation and electronics.

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- Zeng, T. S., W. Zhu, and D. N. Sheng. Two-component Quantum Hall Effects in Topological Flat Bands. 2017. *Physical Review B*. **95**: 125134. <http://10.1103/PhysRevB.95.125134>.

Publications

- Zhu, W., D. N. Sheng, and J. X. Zhu. Magnetic field dependent dynamics and field-driven metal-to-insulator transition of the half-filled Hubbard model: A DMFT plus DMRG study. 2017. *PHYSICAL REVIEW B*. **96** (8): 085118.
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- Wang, L., N. Chepiga, D. K. Ki, L. Li, F. X. Li, W. Zhu, Y. Kato, O. S. Ovchinnikova, F. Mila, I. Martin, D. Mandrus, and A. F. Morpurgo. Controlling the topological sector of magnetic solitons in exfoliated Cr_{1/3}NbS₂ crystals. 2017. *Physical Review Letters*. **118**: 257203. <http://https://doi.org/10.1103/PhysRevLett.118.257203>.

Dynamic Strength and Phase Transition Kinetics in Geophysical Materials

Arianna Gleason Holbrook
20150707PRD2

Project Description

The project will use a brilliant x-ray laser to examine how geophysical materials change the positions and lattice structure of their atoms in response to shock compression. The resulting information will advance the current level of understanding about how these materials behave in geophysical events, such as asteroid impacts and the dynamics of the earth's molten iron core. Understanding the behavior of matter during extreme shocks is directly relevant to the nuclear weapons program.

W. L. Mao. Ultrafast visualization of crystallization and grain growth in shock-compressed SiO₂. 2015. *Nature Communications*. **6**: 8191.

Briggs, M. G. Gorman, A. L. Coleman, R. S. McWilliams, E. E. McBride, McGonegle, J. S. Wark, Peacock, Rothman, S. G. Macleod, C. A. Bolme, A. E. Gleason, G. W. Collins, J. H. Eggert, D. E. Fratanduono, R. F. Smith, Galtier, Granados, H. J. Lee, Nagler, Nam, Xing, and M. I. McMahon. Ultrafast X-Ray Diffraction Studies of the Phase Transitions and Equation of State of Scandium Shock Compressed to 82 GPa. 2017. *PHYSICAL REVIEW LETTERS*. **118** (2).

Publications

Nagler, B., A. Schropp, E. Galtier, B. Arnold, S. Brown, A. Fry, A. Gleason, E. Granados, D. Samberg, F. Seiboth, F. Tavella, Z. Xing, H. J. Lee, and C. Schroer. The phase contrast imaging instrument at the Matter in Extreme Condition endstation at LCLS. 2016. *Review of Scientific Instruments*. **87**: 103701.

Gleason, A., C. Bolme, H. J. Lee, B. Nagler, E. Galtier, R. Kraus, R. Sandberg, W. Yang, F. Langenhorst, and W. Mao. Time-resolved diffraction of shock-released SiO₂ and diaplectic glass formation. 2017. *Nature Communications*. **8**: 1481.

Reagan, M., A. Gleason, L. Daemen, Y. Xiao, and W. Mao. High pressure behavior of the polymorphs of FeOOH. 2016. *American Mineralogist*. **101**: 1483-1488.

Shahar, A., E. Schauble, R. Caracas, A. Gleason, M. Reagan, Y. Xiao, and J. Shu. A pressure effect on iron partitioning in iron alloys. 2016. *Science*. **352**: 580-582.

Gleason, A. E., C. A. Bolme, Galtier, H. J. Lee, Granados, D. H. Dolan, C. T. Seagle, Ao, Ali, Lazicki, Swift, Celliers, and W. L. Mao. Compression Freezing Kinetics of Water to Ice VII. 2017. *PHYSICAL REVIEW LETTERS*. **119** (2).

Brown, S., A. Hashim, A. Gleason, E. Galtier, I. Nam, Z. Xing, A. Fry, A. MacKinnon, B. Nagler, E. Granados, and H. J. Lee. Laser shock drive capabilities at the Matter in Extreme Conditions hutch of the Linac Coherent Light Source. 2017. *Review of Scientific Instruments*. **88**: 105113.

Gleason, A. E., C. A. Bolme, H. J. Lee, B. Nagler, E. Galtier, D. Milathianaki, J. Hawreliak, R. G. Kraus, J. H. Eggert, D. E. Fratanduono, G. W. Collins, R. Sandberg, W. Yang, and

New Nanomaterials with Confined Oxide/Metal Interfaces for Flexible Electrodes

Aiping Chen
20170610ECR

Project Description

Flexible electronics have a huge impact on many applications, from health care to wearable devices. The goal of this project is the design and synthesis of new electrodes with high optical transmission, electrical conductivity, and mechanical stress for the future electronics. This directly addresses the laboratory's grand challenge in materials science. This research not only advances the fundamental understanding of oxide/metal deformation mechanisms, it further provides a unique approach to integrate enhanced mechanical performance and functional properties for applications in future flexible electronics. This research will enable the flexible sensors and functional devices for wearable applications from daily life to the battlefield.

Publications

Shen, L., L. Wu, Q. Sheng, C. Ma, Y. Zhang, L. Lu, J. Ma, J. Ma, J. Bian, Y. Yang, X. Lu, A. P. Chen, M. Liu, H. Wang, and C. L. Jia. Epitaxial Lift-off of Centimeter-Scaled Spinel Ferrite Oxide Thin Films for Flexible Electronics. 2017. *Advanced Materials*. **29**: 1702411.

Joint Mapping of Charge and Spin Degrees of Freedom in Intermediate Valence Materials

Marc Janoschek
20170674PRD2

Project Description

In normal metals, the electrons that conduct electricity do not interact with each other and can be described like the atoms in a gas. However, our recent work and the work of others shows that in functional materials such as plutonium the electrons interact strongly, and more importantly that these strong electronic correlations are crucial for understanding functional material properties. Strong electronic correlations are challenging to measure quantitatively, but in this project, we will establish methods that will allow making significant progress in imaging electronic correlations.

Continuous In-situ Tuning and Nuclear Magnetic Resonance (NMR) Spectroscopy of Correlated Matter

Eric Bauer
20170204ER

Project Description

This project aims to perform nuclear magnetic resonance measurements under continuous in-situ strain to understand the exotic quantum states of matter, such as superconductivity. These unusual states of matter elucidated by our experiments may be used in future energy-saving technologies. For instance, some of the superconducting materials we will study in this project are already being planned for use as the main component, the magnet, in new and improved Magnetic Resonance Imaging machines, which operate at a fraction of the costs of today's machines. The knowledge that we generate in our project may also lead to improved devices under strain conditions that make up the DOE x-ray User Facilities and other high-energy colliders (such as the Large Hadron Collider, which led to the discovery of the Higgs Boson and a Nobel Prize) used throughout the US and the world.

Publications

- Dioguardi, A. P., P. Guzman, P. F. S. Rosa, N. J. Ghimire, S. E. Brown, J. D. Thompson, E. D. Bauer, and F. Ronning. Nuclear magnetic resonance investigation of the novel heavy fermion system $\text{Ce}_2\text{CoAl}_7\text{Ge}_4$. To appear in *Physical Review B*.
- Chan, M. K., R. D. McDonald, J. B. Betts, A. Shekhter, E. D. Bauer, and N. Harrison. Quantum criticality at the charge density wave phase-boundaries in the high- T_c superconductor $\text{HgBa}_2\text{CuO}_{4+\delta}$. Submitted to *Nature Physics*.

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.

On the Origin of Colossal Ion Conductivity

Edward Holby
20160655PRD2

Project Description

This work focuses on understanding how mechanical strain and chemical diffusion are coupled and how layering materials can lead to changes in diffusion properties. This understanding will allow for tailored materials for solid oxide fuel cell membranes. An analytical dipole theory based model will be developed for stress mediated oxygen diffusion, including diffusion through epitaxial layers. Application of these models will yield highly tuned oxide materials structures with improved oxygen conductivity ideal for solid-oxide fuel cell membranes.

Modeling of Two-Dimensional Materials and Hybrid Perovskite Optoelectronic Devices

Sergei Tretiak
20170686PRD3

Project Description

This project involves theoretical modeling of novel layered and three-dimensional materials such as hybrid perovskites. These are promising materials for applications in the area of green energy technologies, such as photovoltaics and water splitting, as well as gamma- and x-ray detector devices pertinent to the core DOE/NNSA missions. Insights gained in this theoretical research will help guiding materials design and fabrication efforts towards applications.

Publications

Zhou. , Zhuo, Kou, Du, and Tretiak. Computational Dissection of Two-Dimensional Rectangular Titanium Mononitride TiN: Auxetics and Promises for Photocatalysis. 2017. *NANO LETTERS*. **17** (7): 4466-4472.

Liu. , Zhou, Tretiak, and Wu. Two-dimensional hexagonal M₃C₂ (M = Zn, Cd and Hg) monolayers: novel quantum spin Hall insulators and Dirac cone materials. 2017. *JOURNAL OF MATERIALS CHEMISTRY C*. **5** (35): 9181-9187.

Engineering Deoxyribonucleic Acid (DNA) Protected Silver Nanoclusters via Doping and Alloying

Jennifer Martinez
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.

Pellet Cracking during Fabrication of Plutonium-238 Oxide Fuel

Adam Parkison
20170531ER

Project Description

The fabrication process currently utilized for the production of $^{238}\text{PuO}_2$ fuel pellets for radioisotope thermoelectric generators (RTG) has a 20-30% pellet failure rate, largely a result of pellet cracking during the fabrication process. This study will produce a MOOSE/BISON simulation of an off-stoichiometric surrogate system as well as the stoichiometric $^{238}\text{PuO}_2$ pellet/clad system.

Insensitive High Explosives using 3-picrylamino-triazole (PATO)

Philip Leonard
20170587ER

Project Description

The development of insensitive high explosives (IHE) that can replace existing explosives in nuclear and other weapon systems is essential in order to improve the safety of US assets without compromising effectiveness. The challenge of generating consistent explosive formulations over decades from domestic materials has driven us to explore new explosives and binders that benefit from economy as well as safety and effectiveness; picrylamino-triazole (PATO) is an excellent material example of these characteristics.

Direct Electrolytic Reduction of Plutonium Oxide Surrogates

Jay Jackson
20170558ER

Project Description

We are developing an electrochemical method to produce plutonium metal in support of a laboratory mission. Our less labor intensive, more efficient and safer process will result in large cost savings and contaminated waste reduction. This project will simultaneously provide valuable data to programs interested in characterization and detection, as well as science of signatures. Additionally, developing the capability in the plutonium facility will facilitate future safeguard studies that can assist with safeguard development in molten salt reprocessing flowsheets, and molten salt reactor designs.

Publications

Monreal, M. J., J. M. Jackson, and K. R. Weisbrod. Electrolytic oxide reduction (EOR). Presented at *NA-532 Information Exchange*. (Nevada Support Facility, Las Vegas, NV, 9-10 Aug. 2017).

Parker, S. S. SEM image of CaSnO₃ crystal growth. Submitted to *Materials Today*.

Chen, C. F., K. R. Weisbrod, M. J. Monreal, E. L. Tegtmeier, and J. M. Jackson. Processing and characterization of Polycrystalline CaRuO₃ Ceramic. Submitted to *Journal of Materials Science*.

Monreal, M. J., J. M. Jackson, and K. R. Weisbrod. Direct electrolytic reduction of plutonium oxide surrogates. Presented at *41st Actinide Separations Conference*. (Chicago, 23-25 May 2017).

Jackson, J. M., M. J. Monreal, and K. R. Weisbrod. Electrolytic oxide reduction (EOR) of plutonium oxide surrogates and the path to plutonium. Presented at *JOWOG 22/2 Focused Exchange Meeting*. (Y-12, Oak Ridge, TN, 18-22 Sept. 2017).

Driven Quantum Matter

Alexander Balatsky
20170665ER

Project Description

The hypothesis that drives this research is that the highly tunable quantum matter (electronic liquid, spins, lattice) will develop qualitatively different responses depending on the nature of the time dependent drives. The ideal outcome of this project would be the test of the central hypothesis: the nature of the induced states in driven quantum matter depends on the nature of external drive: scalar, vector or tensorial. As an intermediate goal we expect to have a catalogue of possible collective instabilities, such as transient excitonic and superconducting instabilities in Dirac Materials (DM) and in Majorana states. We expect the following efforts and results over the project lifetime: 1) Investigation of the mass quench in Dirac materials and Quantum mechanical modeling of the Majorana states quench in topological superconductors. 2) Development of the models to test the role of the dynamics of DM in response to vector fields like magnetic and electric field and modeling of the Dynamical Quantum Phase transitions in Majorana and Dirac states. 3) Demonstration of control of collective instabilities and emergent new collective states in drive DM and Majorana states.

Publications

Huang, , Zhu, D. P. Arovas, Zhu, and A. V. Balatsky. Invariance of Topological Indices Under Hilbert Space Truncation. 2018. *PHYSICAL REVIEW LETTERS*. **120** (1).

Quantum Molecular Dynamics of Strongly Correlated Materials

Kipton Barros
20170450ER

Project Description

Molecular dynamics (MD) simulations have become a powerful and widely used predictive tool in computational materials science, chemistry and biology. MD is also a capability required for a large number of DOE/NNSA missions. Examples include the design of next-generation energy harvesting materials, modeling high-energy explosives, modeling decay of weapons systems, etc. The validity of MD simulations is limited by the accuracy of the potential energy function. An emerging research area is quantum-MD, in which first principle quantum mechanical equations determine the electronic states, from which ionic forces are calculated at every MD time-step. This project better incorporates quantum mechanical effects into MD simulation.

Chern, G. W., K. Barros, Z. Wang, H. Suwa, and C. D. Batista.
Semiclassical dynamics of spin density waves. 2017. *ArXiv e-prints*.

Publications

Wulferding, , Kim, Yang, Jeong, Barros, Kato, Martin, O. E. Ayala-Valenzuela, Lee, H. C. Choi, Ronning, Civale, R. E. Baumbach, E. D. Bauer, J. D. Thompson, Movshovich, and Kim. Domain engineering of the metastable domains in the 4f-uniaxial-ferromagnet CeRu₂Ga₂B. 2017. *SCIENTIFIC REPORTS*. **7**.

Wang, , Barros, Chern, D. L. Maslov, and C. D. Batista. Resistivity Minimum in Highly Frustrated Itinerant Magnets. 2016. *PHYSICAL REVIEW LETTERS*. **117** (20).

Chern, , Barros, C. D. Batista, J. D. Kress, and Kotliar. Mott Transition in a Metallic Liquid: Gutzwiller Molecular Dynamics Simulations. 2017. *PHYSICAL REVIEW LETTERS*. **118** (22).

Ferre, , Haut, and Barros. Learning molecular energies using localized graph kernels. 2017. *JOURNAL OF CHEMICAL PHYSICS*. **146** (11).

o. Ozawa, R. y., Hayami, Barros, and Motome. Shape of magnetic domain walls formed by coupling to mobile charges. 2017. *PHYSICAL REVIEW B*. **96** (9).

Lubbers, N., J. S. Smith, and K. Barros. Hierarchical modeling of molecular energies using a deep neural network. 2017. *ArXiv e-prints*.

Dynamics of Nonequilibrium Phase Transitions and Universality

Wojciech Zurek
20170211ER

Project Description

This project is basic research into the fundamental mechanisms of phase transitions: how one phase of matter transforms into another. The theory being developed has implications for atomic and materials physics, and is a unique application of quantum annealing, which is an early and promising form of quantum computing. The experimental tests being developed involve the nanoscale structure of ferroelectric and magnetic materials. These material systems have many applications in electromagnetic sensing, and optoelectronic devices.

Publications

Zwolak, , and W. H. Zurek. Redundancy of einselected information in quantum Darwinism: The irrelevance of irrelevant environment bits. 2017. *PHYSICAL REVIEW A*. **95** (3).

Gardas, , Dziarmaga, and W. H. Zurek. Dynamics of the quantum phase transition in the one-dimensional Bose-Hubbard model: Excitations and correlations induced by a quench. 2017. *PHYSICAL REVIEW B*. **95** (10).

Harnessing Dark Excitons in Carbon Nanotubes through Covalent Doping Chemistry

Stephen Doorn
20170236ER

Project Description

The defect-state emission we will study presents a unique photon source for optically based quantum information processing and data encryption of interest for global security needs that also offers interesting potential for sensing, imaging, and energy conversion applications. This represents new functionality for carbon nanotubes and results from localization of emitting "excitons" at the new defect sites. Localization in turn provides brighter photoluminescence, longer-lived excited states, and single-photon emission behavior. In order to better harness these behaviors, in this project we aim to probe the electronic structure of the new emitting states using low-temperature spectroscopy techniques. Additionally, the dynamic behavior of these states will be probed to understand relaxation mechanisms, provide additional information on electronic structure and to evaluate how optically generated excitons become trapped at defect sites. Each of these behaviors will be correlated to related nanotube structure and defect surface chemistry to drive new strategies for optimizing the chemical functionalization of carbon nanotubes that is the ultimate origin of this new functionality of significant interest.

Publications

He, X., N. F. Hartmann, Ma, Kim, Ihly, J. L. Blackburn, Gao, Kono, Yomogida, Hirano, Tanaka, Kataura, H. a. n. Htoon, and S. K. Doorn. Tunable room-temperature single-photon emission at telecom wavelengths from sp³ defects in carbon nanotubes. 2017. *NATURE PHOTONICS*. **11** (9): 577-+.

Hartmann, N. F., K. A. Velizhanin, E. H. Haroz, Kim, Ma, Wang, H. a. n. Htoon, and S. K. Doorn. Photoluminescence Dynamics of Aryl sp³ Defect States in Single-Walled Carbon Nanotubes. 2016. *ACS NANO*. **10** (9): 8355-8365.

He, X., B. J. Gifford, N. F. Hartmann, R. Ihly, X. Ma, S. V. Kilina, Y. Luo, K. Shayan, S. Strauf, J. L. Blackburn, S. Tretiak, S. K. Doorn, and H. Htoon. Low-temperature single carbon nanotube spectroscopy of sp³ quantum defects. To appear in *ACS Nano*.

Hybrid Photonic-Plasmonic Materials: Toward Ultimate Control Over the Generation and Fate of Photons

Jennifer Hollingsworth
20170001DR

Project Description

21st-century communication, quantum information and energy-efficient lighting technologies depend on our ability to create, manipulate and detect the basic unit of light: photons. We are developing novel hybrid materials for unprecedented control over these processes. Technological competitiveness in these areas is a national security challenge, as the enabled applications address defense, industrial, and energy security needs, including advanced photodetectors and sensors, secure communications, next-generation computing, and efficient lighting/display technologies. In this way, the fundamental science questions being addressed are "use-inspired," driven by a need to make better and unprecedented use of light in advanced technologies that will underpin our physical and economic security in the coming century. Beyond foundational science, we are developing new tools and capabilities for designing and creating functional hybrid materials. The latter enable precision integration and advanced manufacturing over a range of lengthscales from the nanoscale, where many new important properties emerge, to the macroscale, where real-world applications happen. For example, we are developing techniques for placing single light-emitters into metallic antenna to create novel single and entangled-photon sources for secure communication or sensor qualification, and optical circuitry to remove bottlenecks in communication networks. Integration is at the nanoscale but effects are realized in micro/microscale networks.

Publications

- Dawood, F., J. Wang, C. J. Sheehan, P. A. Schulze, M. R. Buck, A. M. Dennis, S. Majumder, I. Staude, I. Brener, N. A. Amro, and J. A. Hollingsworth. The Role of Liquid Ink Transport in the Direct Placement of Quantum Dot Emitters onto Sub-Micron Antenna by Dip-Pen Nanolithography. Submitted to *Small*.
- Sun., Saxena, and N. A. Sinitsyn. Nearly optimal quantum control: an analytical approach. 2017. *JOURNAL OF*

PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS. **50** (17).

- Li., Sun, V. Y. Chernyak, and N. A. Sinitsyn. Multistate Landau-Zener models with all levels crossing at one point. 2017. *PHYSICAL REVIEW A*. **96** (2).
- Matsuzaki., Vassant, Liu, Dutschke, Hoffmann, Chen, Christiansen, M. R. Buck, J. A. Hollingsworth, Goetzinger, and Sandoghdar. Strong plasmonic enhancement of biexciton emission: controlled coupling of a single quantum dot to a gold nanocone antenna. 2017. *SCIENTIFIC REPORTS*. **7**.
- Peer, A., Z. Hu, A. Singh, J. A. Hollingsworth, R. Biswas, and H. Htoon. Photoluminescence Enhancement of CuInS₂ Quantum Dots in Solution Coupled to Plasmonic Gold Nanocup Array. 2017. *Small*. **13**: 1700660.
- Singh, A., H. D. Magurudeniya, C. Hanson, J. A. Hollingsworth, and M. A. Firestone. Self-assembly directed organization of quantum dots during ionic liquid crystalline polymer formation. Submitted to *Macromolecules*.
- He., N. F. Hartmann, Ma, Kim, Ihly, J. L. Blackburn, Gao, Kono, Yomogida, Hirano, Tanaka, Kataura, H. a. n. Htoon, and S. K. Doorn. Tunable room-temperature single-photon emission at telecom wavelengths from sp(3) defects in carbon nanotubes. 2017. *NATURE PHOTONICS*. **11** (9): 577-†.
- Kwon, H., M. Kim, M. Nutz, N. F. Hartmann, V. Perrin, B. Meany, M. S. Hofmann, C. W. Clark, H. Htoon, S. K. Doorn, A. Hoegeler, and Y. Wang. Ultra-Bright Trions Observed at Fluorescent Quantum Defects. Submitted to *Nature Photonics*.
- Li, H., A. Piryatinski, J. Jerke, A. R. S. Kandada, C. Silva, and E. R. Bittner. Probing dynamical symmetry breaking using quantum-entangled photons. To appear in *Quantum Science and Technology*. <http://arXiv:1707.03304>.
- Welch, P. M., K. O. Rasmussen, and C. F. Welch. Game Theory as a Driver for Non-Equilibrium Dynamics in Soft Matter. Submitted to *Scientific Reports*.
- Sinitsyn, N. A. Computing with a single qubit faster than the quantum speed limit. Submitted to *Physics Letters A*. <http://arXiv/1701.05550>.

- He, X., B. Gifford, N. F. Hartmann, R. Ihly, X. Ma, S. Kilina, Y. Luo, K. Shayan, S. Strauff, J. L. Blackburn, S. Tretiak, S. K. Doorn, and H. Htoon. Low-Temperature Single Carbon Nanotube Spectroscopy of sp^3 Quantum Defects. To appear in *ACS Nano*.
- Ma, , A. R. James, N. F. Hartmann, J. K. Baldwin, Dominguez, M. B. Sinclair, T. S. Luk, Wolf, Liu, S. K. Doorn, H. a. n. Htoon, and Brener. Solitary Oxygen Dopant Emission from Carbon Nanotubes Modified by Dielectric Metasurfaces. 2017. *ACS NANO*. **11** (6): 6431-6439.
- Hanson, C. J., N. F. Hartmann, Singh, Ma, W. J. I. DeBenedetti, J. L. Casson, J. K. Grey, Y. J. Chabal, A. V. Malko, Sykora, Piryatinski, H. a. n. Htoon, and J. A. Hollingsworth. Giant PbSe/CdSe/CdSe Quantum Dots: Crystal-Structure-Defined Ultrastable Near-Infrared Photoluminescence from Single Nanocrystals. 2017. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*. **139** (32): 11081-11088.

Meta-surface Enabled Passive Radiative Cooling

Matthew Reiten
20170357ER

Project Description

The "Meta-Cooler" concept will address national energy security by reducing resources and costs for maintaining a cooled environment for people, electronics, and possibly solar panels in locations exposed to the open sky. A low-cost radiative meta-surface cooler ("Meta-Cooler") will use low-cost engineered materials to reduce the temperature of structures below ambient temperature by enhancing thermal emission while reducing solar spectrum absorption. To circumvent the green house effect, which normally traps and reradiates thermal energy back at hot surfaces, the Meta-Cooler's thermal emissions will be vented into atmospheric "infrared windows." The extra heat will be radiated away into space. Low-cost materials and additive manufacturing will ultimately enable the scale-up of this proof-of-concept to widespread applications. The Meta-Cooler will have broad impact and a wide customer base, including commercial and residential structures and vehicle exteriors. It could assist in force sustainment and humanitarian efforts by reducing the logistics demands of cooling deployable shelters. External heat exchange units coated with Meta-Cooler surfaces could operate with increased efficiency generating significant cost savings.

Hetero-Interfaces of Novel 2D Dirac Semiconductors

Nikolai Sinitsyn
20170328ER

Project Description

Bi-layer transition-metal dichalcogenides materials are extremely interesting for the variety of tunable optical, thermal, and electric properties that they can have depending on relative orientation of different single atomic layers. Los Alamos has the world's highest magnetic field setup to study characteristics of these systems. We want to place the Laboratory as the leading institution to study physical properties of these materials. We hope to observe so-called indirect excitons that are electron-hole bound states. In bilayers, such quasi-particles can have unusually long life-times. Since they carry energy and since they are created by light, there are potential applications in photovoltaics and other optoelectronic and energy efficient applications.

Publications

Stier, A. V., N. P. Wilson, Clark, Xu, and S. A. Crooker. Probing the Influence of Dielectric Environment on Excitons in Monolayer WSe₂: Insight from High Magnetic Fields. 2016. *NANO LETTERS*. **16** (11): 7054-7060.

Keyshar, , Berg, Zhang, Vajtai, Gupta, C. K. Chan, T. E. Beechem, P. M. Ajayan, A. D. Mohite, and Ohta. Experimental Determination of the Ionization Energies of MoSe₂, WS₂, and MoS₂ on SiO₂ Using Photoemission Electron Microscopy. 2017. *ACS NANO*. **11** (8): 8223-8230.

Berg, , Keyshar, Bilgin, Liu, Yamaguchi, Vajtai, Chan, Gupta, Kar, Ajayan, Ohta, and A. D. Mohite. Layer dependence of the electronic band alignment of few-layer MoS₂ on SiO₂ measured using photoemission electron microscopy. 2017. *PHYSICAL REVIEW B*. **95** (23).

Designing Emergent Behavior in the Collective Dynamics of Interacting Nano-Magnets

Cristiano Nisoli
20170147ER

Project Description

Magnetism is critical to areas of national security, from magnetic sensing/control, to information technology, to energy-efficient devices. However, magnets with useful properties at room temperature are rare overall, found serendipitously, and their supply depends on foreign countries. A far greater set of magnetic functionality could be unlocked if we could implement artificial, topologically complex magnetism. Magnetic technology generally concerns itself with manipulation of localized dipolar degrees of freedom, artificial materials containing delocalized monopolar charges, and generally controllable emergent behaviors at room (or desired) temperature is scientifically very exciting but also a possible technological game-changer.

Publications

Mahault, , Saxena, and Nisoli. Emergent inequality and self-organized social classes in a network of power and frustration. 2017. *PLOS ONE*. **12** (2).

Nisoli, , Kapaklis, and Schiffer. Deliberate exotic magnetism via frustration and topology. 2017. *NATURE PHYSICS*. **13** (3): 200-203.

Le, B. L., Park, Sklenar, G. -. Chern, Nisoli, J. D. Watts, Manno, D. W. Rench, Samarth, Leighton, and Schiffer. Understanding magnetotransport signatures in networks of connected permalloy nanowires. 2017. *PHYSICAL REVIEW B*. **95** (6).

Nisoli, C. Write is as you like it. To appear in *Nature Nanotechnology*.

Libal, , Nisoli, Reichhardt, and C. J. O. Reichhardt. Dynamic Control of Topological Defects in Artificial Colloidal Ice. 2017. *SCIENTIFIC REPORTS*. **7**.

Nisoli, C. TOPOLOGY BY DESIGN IN MAGNETIC NANO-MATERIALS: ARTIFICIAL SPIN ICE. To appear in *Topological Materials (Springer Verlag)*. Edited by Saxena, A.

Lao, Y., P. Schiffer, and C. Nisoli. Classical Topological Order in the Kinetics of Artificial Spin Ice. To appear in *Nature Physics*.

Libal, A., C. Reichhardt, C. J. O. Reichhardt, P. Tierno, A. Ortiz, and C. Nisoli. Spin Ice Fragility via Topological Charge Transfer in Artificial Colloidal Ice. Submitted to *Nature Physics*.

Nisoli, C., and R. P. Loreto. Nature Communications. Submitted to *Geometrothermodynamics in planar artificial spin ices*.

Reichhardt, C., A. Libal, C. J. Reichhardt, and C. Nisoli. The Inner Phases of Colloidal Kagome Ice. To appear in *Physical Review Letters*.

Material Processing to Performance: A Path to Physically-Based Predictive Capability

George Gray
20170033DR

Project Description

The ability to numerically represent and accurately predict damage and failure in materials remains elusive, despite its importance to the mission of the Laboratory and the defense complex, as well as many industrial applications. Our lack of predictive capability is related to a poor scientific understanding and quantification of the correlations between material processing, microstructure, properties, and performance (PSPP). The novelty and goal of this project is to understand the complex relationship between material processing and microstructure, specifically its affect on key damage nucleation sites like grain, twin, and solidification boundaries. We will determine where and when material failure initiates through the development of innovative statistical models to represent extremes and tails in distributions. Newfound knowledge about the underlying physics and extreme-value modeling will be the basis for a mechanistic based toolset for predicting failure at the macro-scale as function of processing. Los Alamos has a leadership responsibility for understanding and quantifying the scientific basis and predictive modeling capability to support material performance under high strain rate, stress, complex stress states, and shock-loading conditions. This project will directly contribute to advancing the Laboratory's capabilities in the Materials for the Future focus areas of defects and interfaces, manufacturing, and extreme-loading environments.

Publications

Gray III, G. T., V. Livescu, C. P. Trujillo, C. Knapp, J. Carpenter, and D. Jones. Structure / Property (Constitutive and Dynamic Strength / Ductile Damage) Characterization of Additively Manufactured (AM) 316L SS, 304L SS, and Tantalum. Presented at *DynFrac 2017*.(Trondheim, Norway, 11-15 Sept., 2017).

Bronkhorst, C. A., D. J. Luscher, H. M. Mourad, P. W. Marcy, S. A. Vander Wiel, N. K. Bourne, G. T. Gray III, V. Livescu, and E. K. Cerreta. Meso to Macro Mechanics of Metallic Ductile Damage under Dynamic Loading Conditions. Presented at

Society for Engineering Science Annual Technical Meeting. (College Park, MD, 4-6 Oct, 2017).

Bronkhorst, C. A., V. Livescu, D. W. Brown, J. R. Mayeur, L. Capolungo, and S. A. Vander Wiel. Towards Quantifying the Plastic Flow and Structural State of Additively Manufactured Stainless Steels. Presented at *MACH 2017*. (Annapolis, MD, 5-7 April, 2017).

Hahn, E., S. Fensin, and T. Germann. The influence of grain boundary orientation on the strength and failure of tantalum bicrystals. Presented at *APS SCCM 2017*.(St. Louis, MO, 10-13 July, 2017).

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Versino, D., and C. A. Bronkhorst. A Computationally Efficient Ductile Damage Model Accounting for Micro-Inertia. Submitted to *Computational Methods in Applied Mechanics and Engineering*.

Hahn, E., S. Fensin, and T. Germann. Tensile Strength and Failure Mechanisms of Tantalum at Extreme Rates. Presented at *APS SCCM 2017*.(St. Louis, MO, 10-13 July, 2017).

Gray III, G. T., C. M. Knapp, D. R. Jones, V. Livescu, S. Fensin, B. M. Morrow, C. P. Trujillo, D. T. Martinez, and R. Beal. Structure / Property Characterization of Spallation in Wrought and Additively Manufactured Tantalum. To appear in *APS SCCM 2017*.(St. Louis, MO, 10-13 July, 2017).

Ghosh, S., and C. A. Bronkhorst, Editors. Computational Mechanics - special issue Integrated Computational Structure – Material Modeling of Deformation & Failure under Extreme Conditions .

Bronkhorst, C. A., V. Livescu, D. W. Brown, J. R. Mayeur, L. Capolungo, and S. A. Vander Wiel. Quantifying the Structural State of Additively Manufactured Stainless Steels. Presented at *TMS/USACM Thematic Conference on Recent Advances in Integrated Computational and Experimental Methods for Additive Manufacturing*. (Golden, CO, 6-8 Sept., 2017).

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- Bronkhorst, C. A., and S. Ghosh, Editors. International Journal of Fracture - Special Issue Integrated Computational Structure - Material Modeling of Deformation & Failure under Extreme Conditions.
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Chemical Approaches to Stable, Narrow-Bandgap Perovskite Materials

Nathan Smythe
20170393ER

Project Description

This project aims to address national security challenges in the area of energy security, which is an important DOE mission. A recent Basic Energy Science Advisory Committee (BESAC) report entitled “Basic Research Needs to Assure a Secure Energy Future” clearly emphasized the need to rapidly develop new materials that resist degradation due to various conditions, including temperature effects. This report highlights the need to develop methods for solar energy conversion for the production of fuels and electricity. The report also points out, “inorganic materials science today is critically lacking in the knowledge of predictive reaction pathway mechanisms that would allow the design and synthesis of materials with specified reactivity and properties.” Furthermore, the report goes on to say that “a truly integrated basic research approach of theory, modeling, synthesis, validation and testing is required” in order to facilitate “unprecedented control and predictability of properties and reactivity of technically relevant materials.” Within the scope of this project, we will focus on this integrated approach in order to develop more robust materials capable of supporting light-driven chemical transformations and solar energy conversion.

Interfacial Structure Transfer for Direct Band Gap Wurtzite Group-IV Semiconductors

Jinkyoung Yoo
20170121ER

Project Description

The research enables us to prepare a novel phase of group-IV semiconductors, such as silicon (Si) and germanium (Ge), which are dominant materials for most semiconductor device applications. The novel phase has hexagonal crystal structure and direct electronic band gap according to decades-long theoretical predictions. Furthermore, direct band gap group-IV semiconductors are the ideal building blocks for monolithic optoelectronic integrated system because the highly efficient light-emitting characteristics of direct band gap materials make it possible to fabricate an integrated system encompassing light-emitter, transmitter, detector, and processor with a single material. Direct band gap group-IV semiconductor is the "holy grail" of semiconductor-based optoelectronic devices because it hasn't been realized in reproducible and production-compatible manner. The research is being conducted by an integrated approach of predictive materials design led by quantum mechanical modeling and intensive experimental methods, such as chemical vapor deposition of two-dimensional (2D) materials and Si/Ge, nanocharacterizations, and nanofabrications for multi-scale analyses. Our progress has demonstrated that production-compatible thin film hexagonal Si and Ge can be prepared on 2D materials. The project is closely relevant to the DOE grand challenges to "control at the level of electrons" and "energy and information on the nanoscale."

Publications

Yoo, J., T. Ahmed, R. Chen, A. Chen, Y. H. Kim, K. C. Kwon, C. W. Park, H. S. Kang, H. W. Jang, Y. J. Hong, W. S. Yang, and C. H. Lee. Enhanced nucleation of germanium on graphene via dipole engineering. To appear in *Nanoscale*.

Yoo, J. Multi-dimensional semiconductor heterostructures for basic energy sciences. Presented at *2017 Collaborative Conference on Materials Research*. (Seogwipo, 26-30 June 2017).

Shocked Chemical Dynamics in High Explosives

Shawn Mcgrane
20170070DR

Project Description

The research team is performing time resolved measurements of chemical changes in shocked explosives to validate molecular level simulations. This will enable better prediction of explosive performance and safety through improved modeling of the underlying physics. The goal is to change how explosive modeling is performed, starting at the level of chemical response and predicting hydrodynamics. Currently, the research team starts with large-scale hydrodynamics, and fits artificial underlying chemical models. Changing this will increase predictive capability, allowing us to change materials, geometry, and conditions to increase explosive performance.

Publications

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Krishnapriyan, A., P. Yang, A. M. N. Niklasson, and M. J. Cawkwell. Numerical optimization of density functional tight binding models: Application to molecules containing carbon, hydrogen, nitrogen, and oxygen. To appear in *Journal of Chemical Theory and Computation*.

McGrane, S., P. Bowlan, M. Powell, K. Brown, and C. Bolme. Broadband mid-infrared measurements for shock induced chemistry. To appear in *20th Biennial APS Conference on Shock Compression of Condensed Matter*. (St. Louis, 9-14 July 2017).

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"Zero-Threshold Gain" and Continuous-Wave Lasing Using Charged Quantum Dots

Victor Klimov
20170279ER

Project Description

This project is relevant to the Los Alamos Science of Signatures science pillar; by introducing a novel type of highly flexible and versatile gain media, it can lead to the development of new types of lasers for sensing and diagnostics. Solution-processed quantum-dot lasers are uniquely suited for incorporation into various lab-on-a-chip platforms, such as those specifically for detection of chemical and biological threats. This work can potentially lead to the development of inexpensive, ultra-bright light sources, which can be used for the practical implementation of ideas of laser lighting, a topic of direct relevance to the Los Alamos energy security mission.

Publications

- Wu, K., J. Lim, and V. I. Klimov. Superposition Principle in Auger Recombination of Charged and Neutral Multicarrier States in Semiconductor Quantum Dots. 2017. *ACS Nano*. **11** (8): 8437-8447.
- Park, Y., J. Lim, N. S. Makarov, and V. I. Klimov. Effect of Interfacial Alloying versus Volume Scaling on Auger Recombination in Compositionally Graded Semiconductor Quantum Dots. 2017. *Nano Letters*. **17** (9): 5607-5613.
- Wu, K., Y. Park, J. Lim, and V. I. Klimov. Towards zero-threshold optical gain using charged semiconductor quantum dots. 2017. *Nat. Nanotech.*. advanced online publication.

Radiation Effects and Plasma Interactions in Tungsten Based Materials

Stuart Maloy
20160674PRD3

Project Description

The proposed research will develop a fundamental understanding of radiation effects and plasma material interactions in tungsten-based materials, which applies to the development of improved materials for fusion and spallation applications. This work will lay a foundation for understanding materials in fusion conditions and will ultimately lead to the design of new materials. Los Alamos already has existing expertise in materials at irradiation extremes, focusing mostly on fission environments. The proposed research will strengthen these existing capabilities and also further extend the Laboratory's capabilities in fusion materials research.

Publications

- El Atwani, O., E. Martinez Saez, N. Li, and S. A. Maloy. Advanced Material Design for Fusion Applications. 2017. *MST-8: MATERIALS SCIENCE IN RADIATION & DYNAMICS EXTREMES*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-25380>.
- Wang, Y., A. C. Davis, O. El Atwani, Z. Wang, R. P. Doerner, and S. A. Maloy. New Irradiation Capabilities for Fusion Materials R&D. 2017. *MST-8: MATERIALS SCIENCE IN RADIATION & DYNAMICS EXTREMES*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-25149>.
- El-Atwani, O., J. E. Nathaniel, A. C. Leff, B. R. Muntifering, J. K. Baldwin, K. Hattar, and M. L. Taheri. The role of grain size in He bubble formation: Implications for swelling resistance. 2017. *Journal of Nuclear Materials*. **484**: 236-244. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lapr/LAPR-2017-026467>.
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- El Atwani, O., C. Taylor, J. Frishkoff, W. Harlow, E. V. Esquivel, S. A. Maloy, and M. Taheri. Thermal desorption spectroscopy of high fluence irradiated ultrafine and nanocrystalline tungsten: Helium trapping and desorption correlated with morphology. 2017. *MST-8: MATERIALS SCIENCE IN RADIATION & DYNAMICS EXTREMES*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-24924>.
- El-Atwani, O., J. E. Nathaniel, A. C. Leff, J. K. Baldwin, K. Hattar, and M. L. Taheri. Evidence of a temperature transition for denuded zone formation in nanocrystalline Fe under He irradiation. 2017. *MATERIALS RESEARCH LETTERS*. **5** (3): 195-200. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lapr/LAPR-2017-027194>.
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- El Atwani, O., E. V. Esquivel, and S. A. Maloy. Multiscale irradiation effects of tungsten based materials as plasma facing components. 2017. *MST-8: MATERIALS SCIENCE IN RADIATION & DYNAMICS EXTREMES*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-26201>.
- El Atwani, O., E. Aydogan, E. V. Esquivel, M. Efe, Y. Wang, and S. A. Maloy. Detailed Transmission Electron Microscopy Study on Dislocation Loop Rafting in Tungsten. 2017. *MST-8: MATERIALS SCIENCE IN RADIATION & DYNAMICS EXTREMES*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-27884>.
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- El Atwani, O., E. V. Esquivel, J. Weaver, N. A. Mara, and S. A. Maloy. Mechanical Properties, Damage and Morphology Details of Nanocrystalline and Ultrafine Tungsten Exposed to Low Energy Helium and Heavy Ion Irradiation. 2017. *MST-8: MATERIALS SCIENCE IN RADIATION & DYNAMICS EXTREMES*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-26670>.
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Depleted Uranium Oxides Photodiode

Igor Usov
20170143ER

Project Description

The project aims to address national security challenges and impact the DOE mission in several areas. First, discovery of a novel application for depleted uranium oxide (DUO), accumulated as part of the nuclear fuel cycle and nuclear weapons manufacturing, could significantly reduce the large stockpile of low-level nuclear waste and associated costs of its storage. In addition, it would position not only Los Alamos, but also US DOE and NNSA as leaders in innovative nuclear fuel cycle technologies and innovative utilization of nuclear materials. Our preliminary results also indicate that optoelectronics and electronics applications based on DUO have the potential to address numerous limitations of devices based on conventional semiconductors, such as poor stability and performance in high radiation and high temperature environments. This can lead to development of new technologies for national security (e.g., military, intelligence, reconnaissance, etc.) as well as other specialty applications, such as space exploration, robust electronics for nuclear and accelerator facilities, etc.

In-situ, 3D Characterization of Solidification in Metals

John Gibbs
20150709PRD2

Project Description

By developing new and improved methods of characterizing materials, it will be possible to image solidification in metals in three dimensions. This will ultimately lead to a better ability to predict and control the properties of materials. We will develop the capability to do tomography during controlled directional solidification in proton and x-ray beamlines across the U.S. DOE complex. We will probe solidifying metals with a variety of different diagnostic means to access a wide variety of spatial and chemical data. This will lead to an improved ability to compare experiments and simulations and better theories of solidification dynamics, particularly at non-constant solidification front velocity where there is relatively little data. These datasets will give us a better understanding of solidification and will be made available to validate simulation methods, including a microstructure prediction model that is currently being implemented in the advanced simulation and computing (ASC) code Truchas.

Technical Outcomes

The goals of this project were to develop the hardware and software for imaging the solidification of metals in 3D. A furnace that is capable of solidifying metal samples in an x-ray beam path was built and used at the Advanced Photon Source and a state-of-the-art computed tomography reconstruction software package was developed. Project included initial dataset analysis. The furnace capability will remain available either in its current configuration or as an enhanced tomography capability.

Quantum Control of Tailor-designed Photoactive Energetic Materials

Tammie Nelson
20140668PRD2

Project Description

We will continue to develop a new excited state framework for implementation in the non-adiabatic excited state molecular dynamics code to allow description of photochemical reactions in a realistic environment. We will provide novel computational capabilities critical for understanding light-induced dynamics, including realistic size and environment effects, in many technologically relevant materials. Specifically, this will allow us to simulate large molecular systems where full ab-initio calculations are prohibitively expensive, and to describe systems that interact strongly with solvent environments. Such simulations have been done previously for the ground state but were never attempted for excited states due to computational complexity. Control of explosive initiation would be transformational for Laboratory core missions of stockpile safety.

Technical Outcomes

The project provided a new quantum mechanical and molecular mechanical (QM/MM) approach for excited state molecular dynamics in solvent environments. The new capability describes the light-induced response of large molecules that interact strongly with the environment allowing us to model photoactive processes in materials and natural systems and complement experiments. The project increased the understanding of photoactive energetic materials, and lead to new design principles for future high explosives and materials with controllable chemical dynamics.

Publications

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- Franklin-Mergarejo, R., T. Nelson, S. Tretiak, and S. Fernandez-Alberti. Phonon bottleneck and long-lived excited states in pi-conjugated pyrene hoop. 2017. *Physical Chemistry Chemical Physics*.
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- Bjorgaard, J. A., A. E. Sifain, T. Nelson, T. W. Myers, J. M. Veauthier, D. E. Chavez, R. J. Scharff, and Tretiak. Two-Photon Absorption in Conjugated Energetic Molecules. 2016. *Journal of Physical Chemistry A*. **120** (26): 4455-4464.

Enhanced X-Ray Computed Tomography for Plutonium Manufacturing

James Hunter
20170577ER

Project Description

This project focuses on simulation and demonstration for computed tomography (CT) of pit geometries. The same basic methodology is applicable to other high density/atomic number parts. Other possible applications include jet engine components, high-tolerance piping, and other metal items requiring extensive non-destructive testing analysis. In addition, the anticipated increase in inspection requirements for additively manufactured parts also serves to make advancement of this CT technique desirable from a broader applications perspective.

Technical Outcomes

This project showed the feasibility of using a shaped x-ray beam filter to improve the results of three-dimensional x-ray imaging (CAT scan) for metal parts. An ability to simulate the imaging system with this filter was shown and a one dimensional beam filter was demonstrated on a part at LANL's high energy x-ray facility. This demonstration showed a significant improvement in image quality and can be applied to a broad range of parts.

Active Microwave Beam Steering Using A Metasurface Approach

Houtong Chen
20170565ER

Project Description

Global security applications, specifically dominance of the electromagnetic spectrum, require highly directive beams and agile beam steering. This project studied the feasibility of developing novel low-profile multifunctional antennas based on a metasurface concept, with a goal of accomplishing simultaneously microwave beam collimation with high gain and fast active beam steering with a large field of view. For such a purpose we investigated the resonant response of subwavelength resonators integrated with active elements; each of them was addressed to enable voltage-controlled scattering phase, achieving a spatially-variant phase profile in reflection. We designed, simulated, fabricated, and characterized highly reflective metasurface structures with desirable phase dispersion. We further demonstrated phase tuning when the metasurface structures are integrated with varactor diodes, forming the foundation of accomplishing reprogrammable metasurface reflectors for beam collimation and beam steering capability with characteristics of high-speed, light weight, low cost, and easy to deploy.

Technical Outcomes

Through this project, we designed and demonstrated metasurface structures with high reflection and tunable phases from -180 to $+180$ degrees. We achieved this by integrating active elements such as varactor diodes. This project advanced the body of research towards the ultimate goal of realizing active metasurface reflectors for microwave beam steering with arbitrary directions.

Materials Dynamics via Large-Scale Molecular Dynamics and Embedded Scale-Bridging Simulations

Timothy Germann
20150750ER

Project Description

We will use the Trinity supercomputer, exploiting its heterogeneous set of processor types, to design, optimize, and execute large-scale molecular dynamics and embedded task-based scale-bridging materials science simulations. The scientific goal of these simulations is to better understand and model the dynamic response of materials (specifically tantalum), under impact and spall failure. Our computational goal is to evaluate the use of burst buffer nodes for the database query and interpolation that are central to our adaptive sampling scale bridging. The results of this project will improve subsequent simulation codes and computer architecture designs.

Technical Outcomes

In Phase 1, we demonstrated our Tabasco multi-scale physics code at scale using an asynchronous task-based runtime, with Haswell nodes for the compute-intensive material models, and DataWarp "burst buffer" nodes for the on-the-fly construction and query of a fine-scale response database. In Phase 2, we optimized the SPaSM molecular dynamics code for Knights Landing processors, and performed large-scale (~billion-atom) simulations of the shock compression and spall failure of nanocrystalline tantalum, using DataWarp nodes for checkpoint/restart.

Publications

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Enabling Mesoscale Science: Nonlocal Dislocation-Flux Crystal Plasticity under Shock Loading Conditions

Darby Luscher
20140645ER

Project Description

This project aims to develop a new paradigm in modeling the large deformation response of materials to shock conditions that will enable a simulation-based bridge between microstructure details and weapon performance. We will deliver simulation tools built around the mesoscale physics-based nonlocal models of plasticity that will deliver nonlocal modeling strategies without requiring any length-scale parameters to be specified as inputs. Our research will have a critical role in enabling mesoscale science needed for modeling nucleation and evolution of defects at material interfaces.

Technical Outcomes

The primary and most tangible technical outcome from this project is the implementation of the developed framework and models into the Los Alamos National Laboratory, Advanced Simulation and Computing (ASC) computational hydrodynamics code, FLAG. The models are now available for general use within the release version of this code as a prototype. Continued development of the theory and code is supported by laboratory follow-on efforts.

Publications

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Luscher, D., J. Mayeur, H. Mourad, A. Hunter, and M. Kenamond. Coupling continuum dislocation transport with crystal plasticity for application to shock loading conditions. 2016. *International Journal of Plasticity*. **76**: 111-129. <http://www.sciencedirect.com/science/article/pii/S0749641915001254>.

Luscher, D. J., J. R. Mayeur, H. M. Mourad, A. Hunter, and M. A. Kenamond. A coupled dislocation-flux crystal plasticity theory for modeling shock response of single- and poly-

crystals. Presented at *2016 Mach Conference*. (Annapolis, MD, 5-7 April 2016).

Luscher, D. J., J. R. Mayeur, H. M. Mourad, A. Hunter, and M. A. Kenamond. A coupled dislocation flux crystal plasticity model applicable under shock loading conditions. Presented at *2015 Mach Conference*. (Annapolis, MD, 8-10 April, 2015).

Mourad, H. M. Numerical implementation of a crystal plasticity model with dislocation transport for high strain rate applications. Presented at *The 53rd Annual Technical Meeting of the Society of Engineering Science*. (College Park, MD, 2-5 Oct. 2016).

Mayeur, J. R., H. M. Mourad, D. J. Luscher, A. Hunter, and M. A. Kenamond. Numerical implementation of a continuum dislocation dynamics model of single crystal plasticity. Presented at *2015 Mach Conference*. (Annapolis, MD, 8-10 April 2015).

Luscher, D. J., J. R. Mayeur, H. M. Mourad, A. Hunter, and M. A. Kenamond. Continuum transport of dislocations during shock response of crystals. To appear in *24th International Congress of Theoretical and Applied Mechanics*. (Montreal, Canada, August 21-26, 2016). http://www.ictam2016.org/side_program/book_papers_e.shtml.

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Chemistry in Molten Salt Systems under Extreme Conditions

Stephen Yarbrow
20170678ER

Project Description

The thermodynamics of the salt systems used in advanced Molten Salt Reactors are poorly understood. Los Alamos proposes to use expertise, equipment and procedures developed at the Laboratory to study molten salt systems used for plutonium purification/recovery to define and understand the chemistry behind these challenges. This work will provide a deeper understanding to enable safe deployment of advanced Molten Salt Reactors (MSR).

Technical Outcomes

Electrochemical corrosion experiments on Alloy C22, Ni, Cr, NiChrome, and Th at 520°C in the NaCl-MgCl₂ eutectic showed the nickel alloys had the most corrosion resistance. Uranium in the salt increased the corrosion of Alloy C22. Two perovskites, strontium zirconate and strontium cerate, high temperature proton exchange membranes, were tested with the molten salts. Zirconates are candidates for removing tritium from molten salt solutions used in an MSR.

Efficient Carbon Nanotube Growth on Graphene-Metal Surfaces

Enkeleda Dervishi
20130785PRD2

Project Description

The project is aimed at developing new carbon nanomaterial synthesis methods for enhancing their applications in optical studies and for furthering their incorporation into hybrid materials for electronic, graphene-based membranes and energy-related needs. Our primary technical goal is focused on generating large-area graphene heterostructures. The methods we use will result in generation of functional hybrid-carbon nanomaterials of interest for energy storage, electronic, membrane systems and multi-ferroic applications. These may include hybrid quantum dot/graphene materials, graphene/nanowire heterojunctions, and graphene composites with complex oxide thin films.

Technical Outcomes

Large-area graphene sheets were developed as tunable and selective membranes in microfluidic devices for ion transport studies. The morphological properties of graphene, were controlled by optimizing the synthesis parameters including catalyst type, growth temperature and hydrocarbon flow rate. Graphene/Si(Ge) nanowire heterostructures were synthesized for the next-generation Li-ion electrodes. Raman spectroscopy was used as a diagnostic tool for structural characterization and understanding the reaction dynamics of graphene molecules smaller than 2 nm.

Publications

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Aging in Delta Plutonium Alloys: A Fundamental Approach

Franz Freibert
20150057DR

Project Description

We will quantify and understand the radiogenic changes in delta-Pu induced by helium ingrowth, defect accumulation and delta-Pu phase instability as determined by consensus of state-of-the-art experimental, computational and modeling tools. This project will develop a physically sound basis for pit lifetime estimates advancing the understanding of fundamental radiogenic processes in delta-Pu. Because the focus of Defense Science Campaigns is the development of science impacting stockpile performance, an understanding of radiogenic effects in delta-Pu will impact experiment implementation. Because the focus of Directed Stockpile Work is the function of stockpile technology, aging indicators of performance impact could influence programmatic decisions on Pit Reuse and Lifetime Extension Programs and bound thermo-mechanical processing and supporting technological development for better definition of performance margins and uncertainties.

Technical Outcomes

The project goal was to quantify and understand the radiogenic changes in δ -Pu induced by defect accumulation and evolution from consensus of state-of-the-art experimental, computational and modeling tools. The project resulted in numerous unprecedented, groundbreaking experimental and theoretical findings. Project results will contribute to a new basis for pit lifetime estimates that advance the state of knowledge about fundamental radiogenic processes in δ -Pu.

Publications

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A New Approach to Mesoscale Functionality: Emergent Tunable Superlattices

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Project Description

We will exploit the potential of newly discovered magnetic whirls (so called “skyrmions”) as new magnetic building blocks on the mesoscale (10 – 100 nm in size) to enable the design of novel multi-functional materials. In pursuing our objective, we will not only pioneer a new direction for material science at Los Alamos, we will also have the strong potential of transforming research on functional materials. Using our fully integrated modeling-making-measuring loop we will find “design principles” for various mesoscale skyrmion architectures, which will immediately yield designed functionality via their unique properties. In particular, we expect to identify magnetic mesoscale architecture optimized for new memory or sensing applications. Resulting sensing, storage and computing devices are directly relevant for a new generation of defense and nonproliferation technologies, as well as improving information science and technology.

Technical Outcomes

We investigated the emergence of magnetic skyrmion lattices in an integrated modeling-making-measuring approach. This approach revealed the microscopic interactions that generate skyrmions on the mesoscale that allow for functionality on the macroscale. We demonstrated that controlling magnetic anisotropies is the crucial “design rule” in order to stabilize functional skyrmions, and also in finding new skyrmion materials. Using our suite of theoretical and experimental tools, we demonstrated how to optimize skyrmions for future applications.

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Nuclear Science for Signatures, Energy, Security, Environment

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Project Description

This project proposes to advance our understanding of the electronic structure, phase stability, thermodynamics and thermal properties of nuclear materials. Goals for this project include (1) improving our understanding of dynamic behavior of plutonium, uranium, and some of their compounds across pressure, temperature, time, phase space, surfaces and interfaces for nuclear materials, (2) developing advanced chemical separations and synthesis processes and determine their signatures, (3) expanding capabilities in detection, measurement, and analysis of signatures of nuclear and radiological materials to improve understanding of the environmental behavior and signatures of nuclear materials, and (4) expand the use of Pu-242 to enhance understanding of plutonium aging, electronic structure and chemistry with minimal impact from nuclear decay processes.

Technical Outcomes

The Nuclear Science Fellowships for Signatures, Energy, Security, Environment project supported postdoctoral research in nuclear science relevant to Laboratory mission. The technical engagement and project support of a diverse pool of young bright talented individuals led to award-winning work such as M. Ferrier's research on actinium-225 and its use in Targeted Alpha Therapy cancer treatment. These early career researchers became successful scientists and engineer Laboratory hires continuing work in national mission nuclear science and engineering.

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Majorana Fermions for Quantum Information

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20150628ER

Project Description

The goal of our proposal is to provide evidence for the existence of Majorana fermions and manipulate them in a new class of materials: strongly correlated topological insulators. Quantum information processing will enable tremendous applications, from secure communications to exponentially faster computation, which would be otherwise impossible. However, quantum systems are extremely fragile and sensitive to noise or decoherence, and storing and manipulating quantum information reliably is a major challenge of today's science and technology. A Majorana fermions could have a significant impact on national security because they are much less sensitive to noise effects. They can also provide the platform for quantum information processing, which enables computations not possible on a classical computing architecture.

Technical Outcomes

The goal of our project was to provide evidence for the existence and manipulation of Majorana fermions in samarium hexaboride – superconductor devices. We failed to establish proximity induced superconductivity in samarium hexaboride, likely as a consequence of Fermi velocity mismatch. We also searched, unsuccessfully, for topological superconductivity in the Weyl semimetal compound niobium arsenide.

Publications

Ghimire, N. J., Y. Luo, M. Neupane, D. J. Williams, E. D. Bauer, and F. Ronning. Magnetotransport of single crystalline NbAs. 2015. *JOURNAL OF PHYSICS-CONDENSED MATTER*. **27** (15): 152201.

Luo, N. J. Ghimire, E. D. Bauer, J. D. Thompson, and Ronning. 'Hard' crystalline lattice in the Weyl semimetal NbAs. 2016. *JOURNAL OF PHYSICS-CONDENSED MATTER*. **28** (5).

Defect-Induced Emergent Magnetism in (Nonmagnetic) Complex Oxides and their Interfaces

Scott Crooker
20150613ER

Project Description

This project aims to study and reveal the origin of the recently discovered magnetism that emerges in new oxide semiconductors. We will focus on strontium titanate, which is the foundational material in the new field of "complex oxide electronics." The overall technical goal of this project is to study and ultimately reveal the origin of the recently-discovered magnetism and magnetic effects that emerge in many (nominally nonmagnetic) oxide semiconductors. Strontium titanate is the archetypical and foundational material in a new and burgeoning field of "complex oxide electronics." Our plan is to directly compare magnetism and magneto-optical phenomena in strontium titanate grown by bulk (commercial) methods, by pulsed laser deposition, and by molecular beam epitaxy. The ability to control defects will yield new and unique results since the materials we are going to explore will provide us the opportunity to obtain new and/or improved functionalities not obtainable through bulk materials or by simply changing material chemistry.

Technical Outcomes

This project led to the development of new experimental capabilities for measuring magnetization in new materials down to very short time scales (<1 picosecond, or a millionth of a millionth of a second). These capabilities for "time-resolved Faraday rotation", or "TRKR", are based on ultrafast pulsed lasers. They are important because they allow us to directly measure how spin and magnetization develop and evolve in new technologically-relevant materials, such as complex oxides and 2D semiconductors.

Publications

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Rice, W. D., Liu, T. A. Baker, N. A. Sinitsyn, V. I. Klimov, and S. A. Crooker. Revealing giant internal magnetic fields due to spin fluctuations in magnetically doped colloidal nanocrystals. 2016. *NATURE NANOTECHNOLOGY*. **11** (2): 137-142.

Yang, L., N. A. Sinitsyn, W. Chen, J. Yuan, J. Lou, and S. A. Crooker. Long-lived nanosecond spin relaxation and spin coherence of electrons in monolayer MoS₂ and WS₂. 2015. *Nature Physics*. **11**: 830-834. <http://www.nature.com/nphys/journal/v11/n10/full/nphys3419.html>.

Perovskite Solar Cells: The Next Frontier in Energy Harvesting

Aditya Mohite
20150612ER

Project Description

We will establish design principles for the development of high-efficiency, low-cost perovskite-based solar cells to surpass existing silicon-based technologies. We expect to achieve an understanding of the intrinsic source of high photocurrent and voltage in perovskite-based solar cell devices, as well as how the emergent ferroelectric properties of these unique materials can be tuned to surpass current device efficiencies. The proposed work will strengthen our capability in addressing laboratory missions, particularly in the areas of materials development and energy security.

Technical Outcomes

The key technical outcome of this proposal is the scientific understanding of the rational design principles of hybrid perovskite based materials that allowed for tailoring its structural and electronic properties. This led to proof-of-concept results for high-efficiency optoelectronic applications such as flexible photovoltaics, color tunable LEDs, and photodetectors with performance surpassing state-of-the-art devices made from classical semiconductors.

Publications

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High Efficiency, Low-cost Perovskite Solar Cell Modules

Aditya Mohite
20160320ER

Project Description

In this project, we want to demonstrate a thin-film solar cell module made from the novel perovskite thin-films produced at Los Alamos with > 15% efficiency and stability over several years of operation. State-of-the-art solar cells utilize high purity, single crystalline semiconductors to achieve power conversion efficiency (PCE) of ~20% and have dominated the photovoltaic industry. However, high-purity single-crystal growth requires high-temperatures, which manifests as an increase in the cost per efficiency (2.2 \$/W) of the solar module production. Currently, there is no technology that offers high efficiency at low cost. Photovoltaic power generation is a sustainable green technology that utilizes unlimited, clean solar energy to address the global energy crisis. The success of this project is expected to transform the field of cheap low cost thin-film solar cell technology and take the perovskite technology closer to commercialization with a leveled cost of electricity of 6 c/KWh.

Technical Outcomes

The key outcome of this project was the development of a 2 inch x 2 inch solar cell module with 14% power conversion efficiency with >2000 hours of stability. In addition, we also demonstrated solar cells with >13% efficiency on flexible substrates.

Publications

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Liu, B., C. M. Soe, C. C. Stoumpos, W. Nie, H. Tsai, K. Lim, A. D. Mohite, M. G. Kanatzidis, T. J. Marks, and K. D. Singer. Optical Properties and Modeling of 2D Perovskite Solar Cells. 2017. *Solar RRL*. **1** (8).

Mallajosyula, A. T., K. Fernando, S. Bhatt, A. Singh, B. W. Alphenaar, J. Blancon, W. Nie, G. Gupta, and A. D. Mohite. Large-area hysteresis-free perovskite solar cells via temperature controlled doctor blading under ambient environment. 2016. *Applied Materials Today*. **3**: 96-102. <http://info:lanl-repo/lapr/LAPR-2016-024720> .

Tsai, H., W. Nie, J. Blancon, C. Stoumpos, R. Asadpour, B. Harutyunyan, A. J. Neukirch, R. Verduzco, J. J. Crochet, S. Tretiak, L. Pedesseau, J. Even, M. A. Alam, G. Gupta, J. Lou, P. M. Ajayan, M. Bedzyk, M. G. Kanatzidis, and A. D. Mohite. High-efficiency two-dimensional Ruddlesden-Popper perovskite solar cells. 2016. *Nature*. **Online Only** (Online): Online Only. <http://www.nature.com/nature/journal/vaop/ncurrent/full/nature18306.html>.

Controlled Helium Release from Composite Plasma Facing Materials through Interface Design

Yongqiang Wang
20150567ER

Project Description

This project aims to demonstrate a tungsten (W) based plasma-facing material that continually outgasses helium (He) as it is being implanted, thereby preventing He assisted cavity growth and yielding a stable plasma-facing surface. This demonstration will be accomplished by designing and testing a tungsten-metal (W-M) nanocomposite containing interfaces that provide stable pathways for controlled and continuous He outgassing. Successful demonstration of this novel interface design concept will enable breakthrough improvements in the performance of W based plasma-facing materials under fusion-relevant conditions, and the insights gained will become a broader "toolkit" of materials science and engineering methods that may later be used in other fusion and non-fusion related applications where precipitation of impurities play an important role.

Technical Outcomes

In bulk metals, helium precipitates maintain a roughly spherical shape as they grow, eventually wreaking havoc on a material's mechanical integrity. This project demonstrated that confinement within nanoscale metallic layers causes helium precipitates to spontaneously coalesce into elongated, He-filled nanochannels. The implication is that such nanochannels may not damage materials, and may even facilitate "self-healing" by providing easy paths for controlled, continuous helium release.

Publications

Qin, W. J., F. Ren, J. Zhang, X. N. Dong, Y. J. Feng, H. Wang, J. Tang, G. X. Cai, Y. Q. Wang, and C. Z. Jiang. Helium retention in krypton ion pre-irradiated nanochannel W film. To appear in *Nuclear Fusion*.

Qin, W. J., Y. Q. Wang, F. Ren, M. Tang, Q. Fu, G. X. Cai, L. Dong, L. L. Hu, G. Wei, and C. Z. Jiang. Microstructure and hardness evolution of nanochannel W films irradiated by helium in high temperature. Submitted to *Journal of Nuclear Materials*.

Li, N., M. Demkowicz, N. Mara, Y. Q. Wang, and A. Misra. Hardening due to interfacial He bubbles in nanolayered composites. 2016. *MATERIALS RESEARCH LETTERS*. **21663831**: 1110730.

Yuryev, D. V., and M. J. Demkowicz. Modeling growth, coalescence, and stability of helium precipitates on patterned interfaces. 2017. *Modelling and Simulation in Materials Science and Engineering*. **25**: 015003.

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Chen, D., N. Li, D. Yuryev, K. Baldwin, Y. Q. Wang, and M. J. Demkowicz. Self-organization of helium precipitates into elongated channels under confinement within a metal nano-layer. To appear in *Science Advances*.

Chen, D., N. Li, D. V. Yuryev, J. Wen, K. Baldwin, M. J. Demkowicz, and Y. Q. Wang. Imaging the in-plane distribution of helium precipitates at a Cu/V interface. 2017. *Materials Research Letters*. **5**: 335.

Three-Dimensional Porous Nanographene for Highly Efficient Energy Storage

Edward Holby
20150532ER

Project Description

This project aims to develop 3D nitrogen-doped nanographene anode materials with optimized chemical and physical properties. In order to achieve this goal, we propose a multidisciplinary approach that integrates theoretical predictions from density functional theory calculations and nanoscale dynamic simulations with experimental characterization using well-defined nanographene model systems. In turn, nanographene with optimally designed electronic and geometric structures will be realized through molecularly controlled synthetic methods. We expect to understand fundamental reaction mechanisms of lithium on the doped nanographene structures and ultimately, to propose a path forward to designing structurally stable and high-capacity graphene anodes for energy storage applications.

Technical Outcomes

This project achieved the proposed goals and extended to related fields of study. Technical outcomes include (1) the demonstration of atomic scale control of high capacity battery anode materials (and electrocatalysts), and (2) fundamental understanding of these materials at the atomic scale. Additional metrics include a patent application (IDEA 15-00013), four high-impact publications (Advanced Materials, Nano Energy, and Carbon journals), additional publications (2 in final preparation), and 8 presentations at international conferences.

Publications

- Yen, H., H. Tsai, M. Zhou, E. F. Holby, S. Choudhury, A. Chen, L. Adamska, S. Tretiak, T. Sanchez, S. Iyer, H. Zhang, L. Zhu, H. Lin, L. Dai, G. Wu, and H. Wang. Structurally Defined 3D Nanographene Assemblies via Bottom-Up Chemical Synthesis for Highly Efficient Lithium Storage. 2016. *Advanced Materials*. **28** (46): 10250-10256.
- Wu, G., A. Santandreu, W. Kellogg, S. Gupta, O. Ogoke, H. Zhang, H. Wang, and L. Dai. Carbon nanocomposite catalysts for oxygen reduction and evolution reactions:

From nitrogen doping to transition-metal addition. 2016. *Nano Energy*. **29**: 83-110. <http://www.sciencedirect.com/science/article/pii/S2211285516000124>.

Gao, W., D. Havas, S. Gupta, Q. Pan, N. He, H. Zhang, H. Wang, and G. Wu. Is reduced graphene oxide favorable for nonprecious metal oxygen-reduction catalysts?. 2016. *Carbon*. **102**: 346-356. <http://www.sciencedirect.com/science/article/pii/S0008622316301476>.

Shan, C., H. Yen, K. Wu, Q. Lin, M. Zhou, X. Guo, D. Wu, H. Zhang, G. Wu, and H. Wang. Functionalized fullerenes for highly efficient lithium ion storage: Structure-property-performance correlation with energy implications. 2017. *Nano Energy*. **40**: 327-335. <http://www.sciencedirect.com/science/article/pii/S2211285517305098>.

Precision 'Bottom-Up' Fabrication of Non-classical Photon Sources

Jennifer Hollingsworth
20150604ER

Project Description

We will synthetically integrate optimized, three-dimensionally confined quantum emitters within nanowires capable of efficient subwavelength waveguiding. Single-photon sources are needed as building blocks toward next-generation quantum-information technologies. This work aims to establish new single-photon source capabilities for next-generation quantum information technologies, including secure quantum communication, networking, cryptography, computation, and sensing, with low-threshold lasers also useful for next-gen solid-state lighting and conventional communications.

Dot Emitters onto Sub-Micron Antenna by Dip-Pen Nanolithography. Submitted to *Small*.

Technical Outcomes

1. "Giant" quantum-dot (QD) single-photon-emitter/waveguide or antenna integration: Post-synthesis nano-manipulation by a "direct-write" method, dip-pen nanolithography, was elucidated and then applied to achieve coupled functional systems. 2. Toward electrically driven single-photon emission: ZnO nanowire p-n diode was synthesized by novel full metalorganic chemical vapor deposition (MOCVD) method and characterized for light-emitting diode (LED) properties. 3. 'Speeding up' colloidally synthesized quantum emitters: Emergent property was demonstrated for QD-plasmonic "nanocup" coupled system in novel solution-phase.

Publications

- Peer, , Hu, Singh, J. A. Hollingsworth, Biswas, and H. a. n. Htoon. Photoluminescence Enhancement of CuInS₂ Quantum Dots in Solution Coupled to Plasmonic Gold Nanocup Array. 2017. *SMALL*. **13** (33).
- Yoo, , Ahmed, W. e. i. Tang, Kim, Y. J. Hong, Lee, and Yi. Single crystalline ZnO radial homojunction light-emitting diodes fabricated by metalorganic chemical vapour deposition. 2017. *NANOTECHNOLOGY*. **28** (39).
- Dawood, F., P. A. Schulze, J. Wang, C. J. Sheehan, M. R. Buck, A. M. Dennis, S. Majumder, M. Ticknor, I. Staude, I. Brener, N. A. Amro, and J. A. Hollingsworth. The Role of Liquid Ink Transport in the Direct Placement of Quantum

Sub-Grid Meso-Scale Model for Twinning and Slip Processes

Curt Bronkhorst
20150431ER

Project Description

This project will substantially advance our meso-scale computational material science capability. This work is aggressive and, if successful, will increase our ability to model materials behavior and enable science-based design of new materials. We will develop the numerical element to represent the morphological deformation of mechanical twinning in single crystal metallic materials. The kinetic and kinematic theory to represent the mechanism of twinning will be developed and taken from existing work. The theory will be implemented within the context of the new numerical element, coupled with existing theory for dislocation slip processes. These developments can be used directly in weapons calculations in the future (selected regions of interest) or used to motivate the proper high length scale models to enable representation of slip and twinning together in a physically accurate way across the entire weapons system.

Technical Outcomes

In this project, we formulated and implemented a sub-grid finite element framework, capable of representing the processes of dislocation slip and deformation twinning under dynamic loading. A single-crystal plasticity model was used to characterize the material's response, and a stochastic model was employed to compute the twin nucleation probability at grain boundaries. Experimental work was conducted to investigate the dependence of twin nucleation and growth processes on loading conditions, in support of our modeling effort.

Publications

Mourad, H. M., C. A. Bronkhorst, V. Livescu, and I. J. Beyerlein. A multiscale crystal plasticity finite element framework for the representation of slip and deformation twinning in hcp metals. Presented at *XIV International Conference on Computational Plasticity (COMPLAS 2017)*.(Barcelona, 5-7 Sept. 2017).

- Jin, T., H. M. Mourad, C. A. Bronkhorst, and V. Livescu. Finite element formulation with embedded weak discontinuities for strain localization under dynamic conditions. To appear in *Computational Mechanics*.
- Livescu, V., H. M. Mourad, C. A. Bronkhorst, O. F. Dippo, B. G. Ndefru, I. J. Beyerlein, and L. Capolungo. Low strain twin statistics in high-purity titanium. Submitted to *Acta Materialia*.
- Livescu, V., C. A. Bronkhorst, I. J. Beyerlein, H. M. Mourad, M. L. Lovato, and O. F. Dippo. Quantification of twinning for sub-grid mesoscale modeling. Presented at *TMS Annual Meeting & Exhibition*.(Nashville, Feb. 14-18, 2016).
- Mourad, H. M., C. A. Bronkhorst, V. Livescu, E. K. Cerreta, J. N. Plohr, D. J. Luscher, J. R. Mayeur, and G. T. Gray III. Prediction and numerical representation of adiabatic shear banding in metals. Presented at *IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions*. (Baltimore, June 20-22, 2016).
- Bronkhorst, C., H. Mourad, V. Livescu, I. Beyerlein, and O. F. Dippo. A study of twin formation and early stage growth in high-purity titanium. Presented at *MRS Fall Meeting*. (Boston, Nov. 27 - Dec. 2, 2016).
- Mourad, H. M., C. A. Bronkhorst, V. Livescu, J. N. Plohr, and E. K. Cerreta. Modeling and simulation framework for dynamic strain localization in elasto-viscoplastic metallic materials subject to large deformations. 2017. *International Journal of Plasticity*. **88**: 1-26.
- Mourad, H. M., and C. A. Bronkhorst. Finite element simulations of dynamic shear localization in elasto-viscoplastic solids under adiabatic conditions. Presented at *U. S. National Congress of Computational Mechanics*.(San Diego, 26-30 July, 2015).

Higher Order Spin Noise Spectroscopy: from Foundation of Quantum Mechanics to Applications.

Nikolai Sinitsyn
20150504ER

Project Description

This project aims to demonstrate the new material characterization method and use it to explore essentially new physical phenomena, previously unreachable by conventional means including some of the most fundamental problems in science such as the emergence of the macroscopic classical realism from microscopic quantum mechanics. We will work toward determining higher-order correlators of conducting electrons in gallium arsenide and study the higher-order correlations of a solid-state qubit. Our goal is to build a nano-scale sensor for nuclear spin physics.

Technical Outcomes

We developed a novel two-beam spin-noise spectroscopy (SNS) to study heterogeneous spin systems and measured the 3rd and 4th order spin correlators of semiconductor qubit, warm atomic vapor, and ferromagnetic films. We developed a theory to calculate higher spin correlators in solid state and atomic physics. We probed fundamental quantum dynamics and developed alternative measurement techniques to determine qubit coherence time. Finally, we confirmed that decoherence is due to the nuclear spin bath effects.

Publications

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Near-unity, Stable, Scalable Down-conversion of High-power Light Sources

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20160357ER

Project Description

We aim to accelerate the development of a novel class of “giant” quantum dots as replacements for rare-earth down-conversion materials, underpinning advancements in white-light-emitting devices needed for next-generation solid-state lighting. In three research goals, we will solve remaining challenges limiting these otherwise ideal down-conversion materials: (1) Thermal quenching by correlating performance-under-temperature-stress with nanoscale structure for green and red gQDs, (2) Lifetime performance by engineering the LED to limit sources of thermal load, as well as addressing newly-identified detrimental photo-induced charging/field effects, and (3) Nanomaterial reproducibility/scale-up through new parallel-processing/automation strategies. This work addresses the Laboratory's energy security mission.

Technical Outcomes

This project resulted in several successful technical outcomes. We identified three new stable giant quantum dots (gQDs) spanning green and infrared emission. We developed two new strategies for dramatically increasing long-term operational stability of red-emitting gQDs under high photon flux and temperature. We demonstrated a path-forward for the scaling synthesis of complex nanomaterials for practical applications by novel automated reactor system.

Publications

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Hanson, C. J., N. F. Hartmann, Singh, Ma, W. J. I. DeBenedetti, J. L. Casson, J. K. Grey, Y. J. Chabal, A. V. Malko, Sykora, Piryatinski, H. a. n. Htoon, and J. A. Hollingsworth. Giant PbSe/CdSe/CdSe Quantum Dots: Crystal-Structure-Defined Ultrastable Near-Infrared Photoluminescence from Single Nanocrystals. 2017. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*. **139** (32): 11081-11088.

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Discovering Highly Conducting Oxides by Combining High-Pressure and Thin-Film Techniques

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20160646PRD2

Project Description

Through innovative combination of high-pressure characterization and thin-film deposition methods, this research will develop a number of highly conducting materials with extraordinary properties for energy-related and other applications. The overarching goal of this research is to design and develop novel materials with enhanced or emergent properties for energy-related applications by combining high-pressure and thin-film methods. Taking advantage of the local stresses existing between thin films and their substrates, which are equivalent to external pressures, we will stabilize novel, high-pressure phases with desired properties, i.e. high conductivity, in the form of thin films for practical applications. This project addresses fundamental challenges at the interfaces between physics, chemistry and materials science, and its successful execution will have widespread impact on the development of energy devices using advanced composite films.

Technical Outcomes

We prepared TiO₂ and SnO₂ bilayer thin films with high electron transport and metallic behavior by interfacial reconstruction. Moreover, using high-pressure techniques coupled with in-situ synchrotron and property measurements, we revealed significantly improved structural stability, increased electrical conductivity, and enhanced visible-light responsiveness of an organic-inorganic hybrid perovskite via pressure-induced amorphization and recrystallization. These studies lay the foundation for integration of the high pressure and thin film growth techniques for rational design of novel functional materials.

Publications

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Advances in Near-Field Diffraction Analysis

Edward Kober
20170640ER

Project Description

Quantifiable and predictive models for the response of materials subjected to shock-loading is necessary for the efficient development of materials for use in defense and DOE/NNSA applications. Both DOE/NNSA and the DoD are utilizing diffraction measurements at advanced x-ray sources, particularly the Advanced Photon Source (APS) and the Linac Coherent Light Source (LCLS), to characterize the dynamic response of materials under these conditions. The goal of this project was to advance the technology used to analyze the data obtained in these measurements. In particular, the current analysis assumes that the crystalline grains that comprise the samples remain largely intact during the deformation processes. In this exploratory project, the deformation processes that one particular metal (tantalum) undergo were simulated, and the effects on the resulting diffraction data were calculated. Even for small deformation processes, the impacts on the diffraction data were quite significant. This shows that the techniques could be quite sensitive to changes, but that it will be difficult to quantify them.

Technical Outcomes

Molecular dynamics simulations were used to prepare several Ta samples that had been subjected to high strain-rate loading. The resulting deformation processes were then characterized by available techniques and the diffraction spectra of these samples were calculated. Comparisons between the two enabled the assessment of how the deformations impacted the diffraction data. The changes in the diffraction measurements were quite significant and methods for the limited interpretation of the changes were proposed.

Meso-Photonic Materials for Tailored Light-Matter Interactions

Houtong Chen
20150109DR

Project Description

This project addresses key technological gaps in photonics by developing a class of meso-photonic materials that enable designer electromagnetic functionalities and strong light-matter interactions. The resulting compact, lightweight, flexible, and integrated optical elements and optoelectronic devices will impact threat reduction and global security applications, such as flat lens antennas and focal plane array detectors for communications, imaging, and sensing, particularly for space and satellite sensing of nuclear nonproliferation via effluent detection.

Technical Outcomes

We investigated exotic photonic phenomena and functionalities from meta-molecule structures. Our demonstration of a variety of few-layer metasurfaces revealed novel functionality and enhanced performance for photonic applications, such as flat lenses and structures for solar thermophotovoltaics. We also theoretically investigated light-matter interactions in graphene and its family materials, paving the way to applications based on their unique properties. A high-speed hybrid graphene metasurface spatial light modulator has been demonstrated for imaging and communication applications.

Publications

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Additively Manufactured High Explosive Materials with Controlled Mesostructure for Tuned Detonation Performance.

Alexander Mueller
20150742PRD3

Project Description

This work will combine the development of explosive formulations with polymer rheology to develop explosives for use in a 3D printer. The printed parts' performance will be characterized using various tests. We expect to develop a repeatable method of additively manufacturing HE parts for mechanical and performance testing. Using inert materials, the mechanical properties of structures developed using computer simulations will be assessed. After a down-selection of viable candidate structures, the selected structures will be rendered in high explosives by use of the developed additive manufacturing instrumentation. These parts will be performance tested using a unique suite of Los Alamos explosive characterization techniques.

Technical Outcomes

Additive manufacturing (AM) of high explosives has been developed as Los Alamos National Laboratory capability. Samples up to 50 grams and heights of 80mm tall have been printed with consistent internal structure with dimensions on the scale of $\sim 100\mu\text{m}$. New explosive formulations capable of extrusion through $400\mu\text{m}$ nozzles have been created for 3D printing. Explosive charges have been made using AM that display non-isotropic detonation behavior. Shockwave shaping has been demonstrated with complex internal structures.

Publications

Branch, B., A. M. Schmalzer, B. C. Clements, A. Ionita, B. M. Patterson, P. R. Bowden, B. J. Jensen, B. C. Tappan, D. M. Dattelbaum, and A. H. Mueller. Characterizing the dynamic behavior of additive manufactured mesoscale energetic materials LA-CP-17-20212. To appear in *JANNAF Journal of Propulsion and Energetics*.

Manner, V. W., J. D. Yeager, B. M. Patterson, D. J. Walters, J. A. Stull, N. L. Cordes, D. J. Luscher, K. C. Henderson, A. M. Schmalzer, and B. C. Tappan. In situ imaging during compression of plastic bonded explosives for damage modeling. 2017. *Materials*. **10** (6): 637.

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Catalytic Generation of Gas Using Formic and Oxalic Acids for Pressure/Volume Work

James Boncella
20150743PRD3

Project Description

This project is directed toward fundamental understanding of chemistry that may be used to generate gas pressure from a compact source at low temperatures. The pressure can subsequently be used to drive a switch, actuator or some other mechanical device. Because oxalic acid and oxalate are toxic to various organisms (e.g. in humans, kidney stones are metal oxalates), Nature has evolved a class of enzymes to detoxify this harmful material. By understanding how metal compounds can decompose oxalate, we will generate insight into how the class of enzymes known as oxalate decarboxylases function. The chemical insight gained from these studies will advance our knowledge in the general area of metal catalysis as well as offer the potential to develop a practical application. If successful in developing the conversion of oxalic acid to gases, we will be making a contribution to a potential application that we have identified as being important to certain defense programs.

Technical Outcomes

Our proposal sought to increase the rate of gas pressure generation via chemical methods to obviate the need for gas cylinders. This involved catalyst system development concurrent with probing substrate scope to provide a more rapid rate of gas generation. Catalyst development was extremely successful and several viable candidates have been sent to engineering to develop test systems for cylinder replacement. This work has also generated five publications with several more in preparation.

Publications

Tondreau, A. M., B. L. Scott, and J. M. Boncella. A tertiary carbon-iron bond as an (FeCl)₂(I) synthon and the reductive alkylation of diphosphine-supported iron(II) chloride complexes to low-valent iron. 2016. *ORGANOMETALLICS*. **35** (11): 1643-1651.

Tondreau, A. M., and J. M. Boncella. 1,2-Addition of formic or oxalic acid to N-{CH₂CH₂(PiPr₂)}₂-supported Mn(I)

dicarbonyl complexes and the manganese-mediated decomposition of formic acid. 2016. *ORGANOMETALLICS*. **35** (12): 2049-2052.

Tondreau, A. M., R. Michalczyk, and J. M. Boncella. Reversible 1,2-addition of water to form a nucleophilic Mn(I) hydroxide complex: A thermodynamic and reactivity study. To appear in *Organometallics*.

Tondreau, A. M., and J. M. Boncella. The synthesis of PNP-supported low-spin nitro manganese(I) carbonyl complexes. 2016. *POLYHEDRON*. **116**: 96-104.

Anderson, N. H., J. M. Boncella, and A. M. Tondreau. Reactivity of silanes with (tBuPONOP)ruthenium dichloride: Facile synthesis of chloro-silyl ruthenium compounds and formic acid decomposition. 2017. *Chemistry - A European Journal*. **23**: 13617-13622.

Energetic Materials Cocrystal Engineering: Toward Superior Munitions

Philip Leonard
20150623ER

Project Description

Our project will selectively combine explosives on a molecular level to achieve materials with greater power and better safety for the warfighter. Technical goals for this project are to 1) develop and utilize rational crystal engineering strategies to discover cocrystals, and 2) demonstrate superior explosive safety and performance and improved material properties. The first goal has broad relevance to chemistry in general as modification of physical properties is significant to everything from pharmaceuticals to non-linear optical materials. Achieving a rational design process for cocrystallization based on more than intuition is critical to the future of the field. Developing new explosives is no less critical to national security as existing mainstays are being threatened due to environmental concerns.

Technical Outcomes

We have improved upon existing technology in the characterization and analytical interrogation of cocrystals, the application of scalable formative methods to make cocrystals through acoustic mixing, and the discovery of tetrazine-based cocrystals with both good energy content and high lattice energy. We believe this combination of enabling technologies and important new energetic candidates will accelerate the testing and qualification of new materials, providing improved safety and performance in ordnance and munitions.

Publications

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- Bowden, P. R., P. W. Leonard, J. P. Lichtardht, B. C. Tappan, B. L. Scott, and K. J. Ramos. Energetic salt of trinitrophenol and melamine. 2015. In *APS Shock Compression of Condensed Matter*. (Tampa, 14-19 Jun. 2015). p. 6. Tampa, FL: American Physical Society.

Sensing Applications of Perovskites

Aditya Mohite
20170522ER

Project Description

The main objective of this study is to create and investigate interfaces created between hybrid perovskites and classical inorganic complex oxides and perovskites to achieve novel functionalities. The underlying scientific principle is to control the functionality (optical and electrical) of the hybrid perovskites (or any low-dimensional solution processed semiconductor) by tuning the properties such as electric and magnetic polarization, doping, strain and surface dipoles to manipulate and control the functionality. The ability to manipulate and control the properties of the hybrid perovskites by tuning the properties of the complex oxide/perovskite is expected to have tremendous implications for a range of applications.

Technical Outcomes

The main outcome of this project was the discovery of a new method for tuning the photophysical and electronic properties of perovskites by depositing them on polarized substrates, thereby inducing new properties. We were able to tune the optical response from near infrared (IR) range to the visible range by simply tuning the substrate polarization.

Publications

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- Blancon, J. -, Tsai, Nie, C. C. Stoumpos, Pedesseau, Katan, Kepenekian, C. M. M. Soe, Appavoo, M. Y. Sfeir, Tretiak, P. M. Ajayan, M. G. Kanatzidis, Even, J. J. Crochet, and A. D. Mohite. PEROVSKITE PHYSICS Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. 2017. *SCIENCE*. **355** (6331): 1288-1291.

In situ X-ray Imaging and Diffraction to Understand the Mechanics of Initiation Mechanisms in Explosive Single Crystals

Kyle Ramos
20140643ER

Project Description

This project proposes to use new in situ X-ray experiments and multiscale theory and modeling to observe the first steps in the impact-to-detonation sequence in explosives. We will deliver a validated, anisotropic, thermomechanical model of how single crystals in the explosive RDX respond to shock compression. The equation of state will be employed in a single-crystal plasticity model that incorporates deformation mechanisms and phase transformations that have been observed experimentally. Rates for the deformation mechanisms will be parameterized to experimental data. The ability to model deformation processes in explosives pertains directly to explosive initiation and safety, both of which are of considerable importance to NNSA missions.

Technical Outcomes

Impacts on explosive materials can lead to violent reactions. Using a combination of in situ x-ray experiments at the Advanced Photon Source, atomistic simulations, and continuum single crystal plasticity models, we identified how the complex energetic material RDX responds to impacts. Our models accurately capture how the mechanical properties of RDX depend on sensitivity of impact orientation; our resulting models have been used to understand how impacts lead to reactions in explosives.

Publications

Luscher, D. J., F. L. Addessio, M. J. Cawkwell, and K. J. Ramos. A dislocation density-based continuum model of the anisotropic shock response of single crystal α -cyclotrimethylene trinitramine. 2017. *Journal of the Mechanics and Physics of Solids*. **98** (1): 63-86. <http://www.sciencedirect.com/science/article/pii/S0022509616305245>.

Addessio, F. L., D. J. Luscher, M. J. Cawkwell, and K. J. Ramos. A Single-Crystal Model for the High-Strain Rate Deformation of Cyclotrimethylene Trinitramine including Phase

Transformations and Plastic Slip. To appear in *Journal of Applied Physics*.

Hooks, D. E., K. J. Ramos, C. A. Bolme, and M. J. Cawkwell. Elasticity of Crystalline Molecular Explosives. 2015. *PROPELLANTS EXPLOSIVES PYROTECHNICS*. **40** (3): 333-350.

Hooks, D. E., M. J. Cawkwell, and K. J. Ramos. Plasticity in crystalline molecular explosives—A key to unraveling “unpredictable” responses. 2016. *Propellants, Explosives, Pyrotechnics*. **41** (2): 203-204.

Cawkwell, M. J., D. J. Luscher, F. L. Addessio, and K. J. Ramos. Equations of state for the alpha and gamma polymorphs of cyclotrimethylene trinitramine. 2016. *JOURNAL OF APPLIED PHYSICS*. **119** (18).

Dendritic microstructure selection in cast metallic alloys

Damien Tournet
20150713PRD2

Project Description

We will build a multi-scale model for solidification processing that includes fluid flow for the first time, which is critical for predicting metallic alloy microstructural development that controls materials properties and performance. Cutting-edge, multi-scale simulations validated by in situ experiments will shed light on the poorly understood, yet crucial effects of gravity on microstructure selection in metallic alloys during metallurgical processing. Understanding crystal growth under gravity-induced liquid flow across length scales will enable the control of microstructure and defects in cast parts. This project will mark a transformational leap toward reaching predictive capability for advanced manufacturing at Los Alamos, aimed at tailoring materials microstructures and properties relevant to national security and energy challenges. It will also provide new, predictive computational tools needed for future materials-for-the-future studies.

Technical Outcomes

Solidification is the first processing stage experienced by most manufactured parts and can have a profound influence on the microstructure and therefore properties of a material. This relationship is difficult to model due to the vast difference between the length scales of solidification conditions (nanometers) and microstructure (micrometers to millimeters). In this work, a multi-scale dendrite needle network model, which can bridge this gap in scale, was developed and validated against experimental data.

Publications

- Tournet, D., and A. Karma. Three-dimensional dendritic needle network model for alloy solidification. 2016. *Acta Materialia*. **120**: 240-254.
- Tournet, D., J. C. E. Mertens, E. Lieberman, S. D. Imhoff, J. W. Gibbs, K. Henderson, K. Fezzaa, A. L. Deriy, R. A. Lebensohn, B. M. Patterson, and A. J. Clarke. From solidification processing to microstructure to mechanical

properties: A multi-scale X-ray study of an Al-Cu alloy sample. Submitted to *Metallurgical and Materials Transactions A*.

Mota, F. L., Y. Song, J. Pereda, B. Billia, D. Tournet, J. M. Debierre, R. Trivedi, A. Karma, and N. Bergeon. Influence of convection during directional solidification of a bulk transparent alloy: comparison of 1g and μ g experiments performed in the DECLIC-DSI and phase-field simulations in a diffusive growth regime . Submitted to *JOM*.

Tournet, D., Y. Song, A. Clarke, and A. Karma. Grain growth competition during thin-sample directional solidification of dendritic microstructures: A phase-field study. 2017. *Acta Materialia*. **122**: 220-235.

Record-Low Lasing Thresholds Using Colloidal Type-II Quantum Wells

Victor Klimov
20150764PRD4

Project Description

This project seeks to explore the use of engineered colloidal nanomaterials to achieve optical gain at low excitation intensities. The proposed studies will elucidate general design principles for colloidal optical gain media via an integrated approach involving parallel optimization of all nanostructure parameters relevant to lasing performance. The success of this work will provide an important milestone on the way to electrically pumped lasers based on colloidal nanomaterials. Further development of colloidal quantum well materials into low-threshold, electrically pumped, highly tunable lasers can lead to useful remote sensing applications as portable, energy-tunable, coherent excitation sources, with application to national security problems such as nuclear nonproliferation.

Technical Outcomes

In this project, we investigated optical-gain properties of colloidal nanocrystals and explored a new light-amplification scheme based on charged exciton states. By applying charging strategies to quantum dots with a radially-graded composition designed for suppressing nonradiative Auger decay, we were able to reduce the optical-gain threshold by almost two orders of magnitude. Our findings indicate a considerable promise of engineered quantum dots for realizing solution-processable lasing devices operating in both pulsed and continuous-wave regimes.

Publications

- Liu, W., Q. Lin, H. Li, K. Wu, I. Robel, J. M. Pietryga, and V. I. Klimov. Mn²⁺-Doped Lead Halide Perovskite Nanocrystals with Dual-Color Emission Controlled by Halide Content. 2016. *Journal of the American Chemical Society*. **138** (45): 14954-14961.
- Wu, K., Y. S. Park, J. Lim, and V. I. Klimov. Towards zero-threshold optical gain using charged semiconductor quantum dots. Submitted to *Nature Nanotechnology*.

Exploring Conditions for Dislocation Transmission Across Grain Boundaries via Phase Field Dislocation Dynamics

Darby Luscher
20170679ER

Project Description

Material defects and their interactions substantially contribute to the macroscopic mechanical behavior of materials, particularly under dynamic loading. Traditional continuum models have treated these interactions through phenomenological approaches, or through various homogenization schemes. While such approaches have provided insight, the physics governing these interactions, the relevance, and the validity of such approaches all remain important points of scientific inquiry. This project set out to modify and employ a phase field dislocation dynamics (PFDD) model to simulate dislocation transmission across copper symmetric tilt grain boundaries towards the ultimate goal of characterizing this behavior under varying rates of loading. The obtained numerical solutions will aid in the development of an analytic continuum interface model. The computations and model development will lead to a continuum interface theory for the rate of dislocation flux across grain boundaries with respect to far field loading amenable to implementation within existent crystal plasticity and shock hydrocode models.

Technical Outcomes

In this research, we demonstrated that the elastic fields in the crystals on either side of a grain boundary are weakly dependent on the adjacent crystal. Second, we have developed approximate explicit expressions for the displacement, displacement gradient, and stress field within each crystal. Significantly, elastic models which consider the interaction between dislocations and grain boundaries may be augmented by this work with simple analytic expressions which incorporate elastic anisotropy.

Novel Routes to Emergent Functionality in Multiferroics

Vivien Zapf
20150759PRD3

Project Description

This project will lay the critical groundwork for understanding new coupling mechanisms between magnetism and ferroelectricity. We will identify and characterize this coupling in existing and new chemical compounds. Sensors rely on strong coupling between two properties - the property to be sensed and the circuit (generally electric) performing the sensing. Most commercial magnetic sensors such as those used in iPhones and hard drives couple magnetism to electrical transport properties. Unfortunately, most magnetic sensors today use high power and dissipate heat due to the need to drive electrical currents. By switching to ferroelectricity instead of electrical transport we vastly reduce the power consumption by manipulating voltages rather than currents. The longer range goals of this area of research impact sensing and devices. Low-power sensing is a needed technology for distributed in-the-field surveillance as well as numerous technological applications.

Technical Outcomes

We discovered materials with new magnetic and magnetoelectric functionalities including the first-ever use of a spin-state transition to drive multiferroic behavior (the coupling between magnetism and ferroelectricity), a new approach to hysteretic multiferroic behavior, and finally a new record coercive magnetic field at low temperatures. This research is motivated by eventual applications in low-power sensing, alternative energy, tunable frequency devices and low-power approaches to memory and computing.

Publications

Singleton, J., J. W. Kim, C. V. Topping, A. Hansen, E. Mun, S. Chikara, I. Lakis, S. Ghannadzadeh, P. Goddard, X. Luo, Y. S. Oh, S. Cheong, and V. S. Zapf. Magnetic properties of $\text{Sr}_3\text{NiIrO}_6$ and $\text{Sr}_3\text{CoIrO}_6$: Magnetic hysteresis with coercive fields of up to 55 T. 2016. *Phys. Rev. B.* **94**: 224408. <http://link.aps.org/doi/10.1103/PhysRevB.94.224408>.

Brambleby, J., J. L. Manson, P. A. Goddard, M. B. Stone, R. D. Johnson, P. Manuel, J. A. Villa, C. M. Brown, H. Lu, S. Chikara, V. Zapf, S. H. Lapidus, R. Scatena, P. Macchi, Y. Chen, L. Wu, and J. Singleton. Combining microscopic and macroscopic probes to untangle the single-ion anisotropy and exchange energies in an $S=1$ quantum antiferromagnet. 2017. *Phys. Rev. B.* **95**: 134435. <http://link.aps.org/doi/10.1103/PhysRevB.95.134435>.

Chen, C. W., S. Chikara, V. S. Zapf, and E. Morosan. Correlations of crystallographic defects and anisotropy with magnetotransport properties in $\text{Fe}_x\text{Ta}_{1-x}\text{S}_2$ single crystals ($0.23 \leq x \leq 0.35$). 2016. *Physical Review B.* **94**: 054406.

Chikara, S., J. Singleton, J. Bowlan, D. A. Yarotski, N. Lee, H. Y. Choi, Y. J. Choi, and V. S. Zapf. Electric Polarization observed in single crystals of $\text{Lu}_2\text{MnCoO}_6$. 2016. *Physical Review B.* **93**: 180405R.

Ho, P. C., J. Singleton, P. A. Goddard, F. F. Balakirev, S. Chikara, T. Yanagisawa, M. Brian Maple, D. B. Shrekenhamer, X. Lee, and A. T. Thomas. Fermi-surface topologies and low-temperature phases of the filled Skutterudite compounds $\text{CeOs}_4\text{Sb}_{12}$ and $\text{NdOs}_4\text{Sb}_{12}$. 2016. *Phys. Rev. B.* **94**: 205140.

Chikara, S., G. Fabbris, J. Terzic, G. Cao, D. Khomskii, and D. Haskel. Charge partitioning and anomalous hole doping in Rh-doped $\text{Sr}_2\text{MnIrO}_4$. 2017. *Phys. Rev. B.* **95**: 060407. <http://link.aps.org/doi/10.1103/PhysRevB.95.060407>.

Laser Additive Manufacturing of Grade 92 (P92) Steel for Radiation Tolerant Nuclear Components

Thomas Lienert
20170591ER

Project Description

To achieve energy security and reductions in greenhouse gases, the US must develop and deploy clean, affordable, domestic energy sources as soon as possible; nuclear energy is a key component in this strategy. One of the key challenges facing the nuclear energy industry involves development of innovative reactor designs to reduce capital costs. This project focuses on fabricating reactor grid plates of P92 steel, a radiation tolerant steel, using laser additive manufacturing (LAM) is proposed. LAM is particularly well suited for more rapid and economical fabrication of the grid plates. The project involves a study of laser additive manufacturing (LAM) of reactor grid plates of P92 steel with engineered radiation tolerance and increased affordability relative to current practices. This work has potential to transform fabrication methods for reactor components made from radiation-tolerant materials with increased affordability.

Technical Outcomes

This project successfully demonstrated the feasibility of using Additive Manufacturing to produce reactor components. We additively manufactured creep resistant ferritic steels to produce the desired mechanical properties and radiation tolerance to specs better than or equal to wrought materials. A sub-scale prototype of a reactor component was fabricated.

Additive Manufacturing of Hierarchical Multi-Phase High-Entropy Alloys for Nuclear Components

Nan Li
20170578ER

Project Description

In the recently published DOE report “Next Generation Materials: Technology Assessment,” innovative irradiation-resistant steels with lifespans up to 80 years by 2020 have been identified as a critical need. To accomplish this requirement is extremely challenging. It requires us to explore both the materials and the corresponding manufacturing processes. In recent years, high entropy alloys, composed of four or more metallic elements mixed in equal or near equal atomic percent, have attracted significant attention due to their excellent mechanical properties and good corrosion resistance. They show significant promise as candidates for high temperature fission and fusion structural applications. However, the conventional synthesis methods are unlikely to present an industrially suitable route for the production and use of high entropy alloys. Recognizing rapidly evolving additive manufacturing techniques, the motivation of this proposal is to optimize the additive manufacturing process to fabricate hierarchical dual-phase high entropy alloys with pre-designed chemical compositions and phase morphology for nuclear components. In this project, the state-of-the-art synthesis techniques have been synergistically integrated with a learning framework to propose experiments in search of the targeted high entropy alloys.

Technical Outcomes

This project achieved 3 major technical milestones. (1) We investigated FCC FeCrNiMn and BCC FeCrNiMnAl High-Entropy Alloys (HEAs) and found they present comparable swelling and extraordinary irradiation tolerance. (2) We found that microstructure and radiation-induced hardening can be tailored by laser processing under additive manufacturing. (3) We assembled a unique database of HEAs containing a total of 686 experimentally explored multicomponent HEA alloys.

Controlling the Electronic Structure of Emerging Atomically Thin Materials Through Heterostructuring

Jinkyoun Yoo
20150659ECR

Project Description

High-quality semiconductor growth via chemical vapor deposition, nanofabrications for electronic/photonics devices, temperature-dependent electrical transport measurements, and theoretical calculations to estimate materials' properties will be performed. The overarching goal of the research is controlling the physical properties of emerging two-dimensional atomically thin materials (2D-ATM) such as graphene through heterostructure formation with conventional semiconductor (i.e. silicon) growth on 2D-ATMs. The project is directly relevant to the DOE grand challenges to "control at the level of electrons" and "energy and information on the nanoscale." It also provides materials systems composed of ultimately (atomically) thin material and semiconductors of which properties are precisely controlled to tackle the grand challenges.

Technical Outcomes

We achieved development of general growth strategy of heterostructures composed of conventional semiconductors and atomically thin emerging two-dimensional (2D) materials. The advantages of our heterostructures are structural quality without strain and structural defects at the interface regardless of materials combination, tunable electrical characteristics of the heterostructures and individual entities via charge transfer through the interface, enabling novel phase of conventional semiconductors, such as hexagonal germanium, and building blocks of high-performance flexible devices.

Publications

- Lin, Y. -C., I. Bilgin, T. Ahmed, R. Chen, D. Pete, S. Kar, J. -X. Zhu, G. Gupta, A. Mohite, and J. Yoo. Charge Transfer in Crystalline Germanium/Monolayer MoS₂ Heterostructures Prepared by Chemical Vapor Deposition. 2016. *Nanoscale*. **8**: 18675-18681.
- Lin, Y. -C., J. Yoo, I. Bilgin, R. Chen, A. Mohite, S. Kar, D. Pete, and C. Sheehan. Controlling physical properties of two-

dimensional materials through heterostructuring. 2015. *2016 Gordon Research Conference: 2D Materials beyond Graphene*.

Lin, Y. -C., J. Yoo, I. Bilgin, A. Mohite, S. Kar, and D. Pete. Growth and characterizations of germanium/monolayer MoS₂ heterostructures. 2015. *2015 Materials Research Society Spring Meeting*.

New States of Matter in Weyl Semimetals

Brad Ramshaw
20160616ECR

Project Description

Subjecting new materials to extreme environments, such as high magnetic fields, can uncover new quantum-mechanical phenomena. We will develop a pulse-echo ultrasound tool to measure the speed of sound in materials. The ability to resolve material properties in dynamical experiments is of critical importance at Los Alamos. Our proposed pulse-echo ultrasound implementation will be limited only by the speed of sound in the material. For a longitudinal sound wave traveling through a 1 mm sample of aluminum, this translates into elastic modulus measurement with a time resolution of about 200 nanoseconds. Such a capability would be of immediate interest for dynamical materials testing.

Technical Outcomes

The project resulted in a new Pulsed Echo Ultrasound system that is capable of collecting data in a transient and extreme environment with an improved signal to noise ratio 50 times better than the leading competitor's system. The method may be utilized in other transient environments in which material properties govern performance.

A Novel Crystal Plasticity Model that Explicitly Accounts for Energy Storage and Dissipation at Material Interfaces

Jason Mayeur
20150696ECR

Project Description

This project will develop a simulation tool that can be used to better understand the performance of existing nanostructured metallic material systems and guide the design of next-generation systems with microstructures tailored for specific applications. A primary goal is to develop a nonlocal crystal plasticity model to study the competition between bulk-dominated and interface-dominated polycrystalline plasticity at the mesoscale. The model will be used to study the mechanical response of nanocrystalline face-centered cubic (fcc), body-centered cubic (bcc), and fcc/bcc lamellar composites. It is anticipated that the improved understanding of these nanoscale material systems obtained via simulation will facilitate next-generation materials design by identifying relationships between process parameters and the resulting microstructure.

Technical Outcomes

This project developed a novel grain scale theory and computational model for studying the thermomechanical response of nanocrystalline metals and composites. Simulations using the newly developed model led to an enhanced understanding of the interplay between intragranular and interfacial plasticity in Cu-Nb lamellar nanocomposites. This understanding provided insight into the origin of their exceptional mechanical properties, beyond what simple rule-of-mixtures had predicted.

Publications

- Mayeur, J. R., and D. L. McDowell. Micropolar crystal plasticity simulation of particle strengthening. 2015. *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*. **23** (6).
- Mayeur, J. R., D. L. McDowell, and S. Forest. Micropolar and Micromorphic Crystal Plasticity. Submitted to *Handbook of nonlocal continuum mechanics for materials and structures*. Edited by Voyiadjis, G. Z.

Uniaxial Pressure to Elucidate Complex Electronic States in Actinides

Filip Ronning
20150702PRD1

Project Description

We will develop a capability to perform nuclear magnetic resonance measurements on actinide-based materials under uniaxial strain. This will help uncover the origin of superconductivity in a variety of actinide superconductors. Specifically, this work will add an important new capability in the field of condensed matter research. Anticipated results include: addressing the microscopic origin of the so-called nematic order in URu₂Si₂, confirming or invalidating the presence of a chiral superconducting order parameter in UPt₃, and possibly revealing the presence of a valence transition in PuCoGa₅ and its role in mediating superconductivity. The response of these materials to uniaxial pressure could help answer major open questions about the nature of the complex electron interactions in a broad class of novel materials.

Technical Outcomes

A novel uniaxial strain cell was developed to perform nuclear magnetic resonance (NMR) measurements under strain. Several strongly correlated electron systems were studied with NMR to better understand their spin fluctuations. Finally, the NMR signal from ²³⁹-plutonium nuclei was observed for only the second time.

Publications

- Dioguardi, A. P., P. Guzman, P. F. S. Rosa, N. J. Ghimire, S. E. Brown, J. D. Thompson, E. D. Bauer, and F. Ronning. Nuclear magnetic resonance investigation of the novel heavy fermion system Ce₂CoAl₇Ge₄. Submitted to *Physical Review B*.
- Kissikov, A. P. Dioguardi, E. I. Timmons, M. A. Tanatar, Prozorov, S. L. Bud'ko, P. C. Canfield, R. M. Fernandes, and N. J. Curro. NMR study of nematic spin fluctuations in a detwinned single crystal of underdoped Ba(Fe_{1-x}Cox)₂As₂. 2016. *PHYSICAL REVIEW B*. **94** (16).

Strain and Dimensional Tuning of Heavy-Fermion Superconductors

Filip Ronning
20160673PRD3

Project Description

The project proposes to develop new capabilities for measuring electronic properties under pressure and in pulsed magnetic fields. The interplay between magnetism and electronic conduction is important for energy security (in the form of superconductivity) as well as information science and technology (by the possible creation of novel excitations which can be platforms for quantum information science). This work will provide new insight into magnetic instabilities and the new states formed there, as well as grow new heavy fermion thin films to understand the role of dimensionality in creating the heavy fermion state.

Technical Outcomes

This project shed light on integrating rich f-electron physics with highly mobile 3d electrons for creating exotic physical phenomena. Films of f-electron materials were grown to investigate new effects at the interfaces. Samarium oxide films were grown on top of strontium titanate. Evidence of interface effects were observed in transport measurements revealing a conducting substrate influenced by the magnetism of the thin film grown on top.

A Dedicated Database Server for f-electron Systems for Actinide Science

Towfiq Ahmed
20170680ER

Project Description

The world has an ever-increasing need for materials with newer electronic functionalities and higher energy efficiency. Over the last century, the physics, chemistry and materials science community has been exhaustively exploring the compounds containing elements from the top half of the periodic table using various theoretical and experimental tools. However the second half, particularly the last-row elements (e.g. actinides) of the periodic table and their compounds, remain under-explored. Although widely known for nuclear energy applications, actinides-based compounds have recently attracted attention for their complex and interesting electronic properties, such as superconductivity and strong magnetism, with numerous national security and energy-related applications. To leverage on these rich electronic properties, and to design new materials, we developed a database with predictive capability for new and enhanced structural and chemical functionalities. With all these different data query and mining tools, our database is uniquely attributed with high-quality, theoretically simulated electronic information. Our database is focused and well equipped for the discovery of next-generation functional materials for national security and energy applications. This project addresses outstanding problems identified by NNSA, the Science Advanced Scientific Computing Research program, and the Scientific Discovery through Advanced Computing program in the area of advanced computing for materials.

Technical Outcomes

This project developed an f-electron structure database (FESD). To achieve this, we verified available data with machine learning algorithms. A key feature of the database is the electronic structure data (bandstructure, DOS) generated from ab initio simulations. We analyzed the atomic-orbital characteristics of bands near the Fermi energy, and additionally predicted the stability of double perovskite super-structures. Finally, we demonstrated the database's efficacy in studying

fundamental electronic interactions of actinide based materials.

Publications

- Hafiz, H., A. I. Khair, H. Choi, A. Mueen, A. Bansil, S. Eidenbenz, J. Wills, J. X. Zhu, A. Balatsky, and T. Ahmed. f-electron structure database (FESD): A data analysis and learning tool for strongly correlated materials . Submitted to *Physical Review Materials*.
- Ardenljan, M., M. Jain, S. Pathak, A. Kumar, N. Li, M. Knezevic, and I. J. Beyerlein. Deformation mechanisms in room temperature deformation of bcc Mg/bcc Nb nanolayered composites. Submitted to *Physical Review B*.

X-ray Split and Delay for Time-Resolved Single Target Shock Compression Studies

Arianna Gleason Holbrook
20170624ER

Project Description

The research team successfully built, tested and benchmarked the first hard X-ray split and delay line with a static delay suitable for shock physics. This unique X-ray diagnostic can follow the passage of a compressive wave through a single-target with unparalleled temporal and spatial resolution enabling the next generation of dynamic compression kinetics experiments. Using diffraction or imaging, it is now possible to track mesoscale material transformation in real-time. The design included single crystal Si optics, (220) and (400) to spatially split and steer the incident X-ray beam to achieve the desired delay of 0.9 nanoseconds. This project produced a fieldable delay-line and dynamic driver.

Technical Outcomes

We have successfully built and benchmarked the first hard X-ray split and delay line with a static delay suitable for shock physics. This X-ray diagnostic will enable us to follow the passage of a compressive wave through a single-target with unparalleled temporal and spatial resolution – critical for measuring mesoscale material transformations in real-time. Our design included single crystal Si optics to spatially split and steer the X-ray beam.

New Physics in New Materials

Priscila Ferrari Silveira Rosa
20150710PRD2

Project Description

The goal of this work is to discover new electronic states and characterize them with the intention of opening an entirely new scientific direction in the quantum physics of materials. Exploring properties of promising new materials at extremes of low temperatures, high pressures and high magnetic fields is a very useful means to uncover new physics. This project proposes to use electrical resistivity and specific heat measurements to study new intermetallic compounds under extreme conditions. The goal is to show that quantum criticality and heavy electron superconductivity can be found in materials without f-electrons and without iron. We will also search for a second example of a heavy electron material that becomes superconducting and subsequently magnetic.

Technical Outcomes

The discovery of new physics in new materials advances our fundamental understanding of materials, and ultimately enables new technologies. We discovered a new magnetic phase driven by magnetic impurities in the quantum material CeRhIn5 at high pressures. Our discovery sheds light on the emergence of intertwined orders and portends possibilities for new states in other materials that host a spin resonance - the particular excitation that induce the observed magnetism.

Publications

- S. Rosa, P. F., Oostra, J. D. Thompson, P. G. Pagliuso, and Fisk. Unusual Kondo-hole effect and crystal-field frustration in Nd-doped CeRhIn5. 2016. *PHYSICAL REVIEW B*. **94** (4).
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- S. Rosa, P. F., J. Kang, Y. Luo, N. Wakeham, E. D. Bauer, F. Ronning, R. M. Fernandes, Z. Fisk, and J. D. Thompson. Competing magnetic orders in the superconducting state of heavy-fermion CeRhIn5. 2017. *Proceedings of the National Academy of Sciences*. **114**: 5384-5388.

- Huang, K., S. Eley, P. F. S. Rosa, L. Civale, R. E. Baumbach, M. B. Maple, and M. Janoschek. Quantum Critical Scaling in the Disordered Itinerant Ferromagnet UCo1-xFexGe. 2016. *Physical Review Letters*. **117** (23): 237202.
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- Wakeham, N., P. F. S. Rosa, Y. Q. Wang, M. Kang, Z. Fisk, F. Ronning, and J. D. Thompson. Low-temperature conducting state in two candidate topological Kondo insulators: SmB6 and Ce3Bi4Pt3. 2016. *Physical Review B*. **94** (3): 035127.
- Laurita, N. J., C. M. Morris, S. M. Koohpayeh, P. F. S. Rosa, W. A. Phelan, Z. Fisk, T. M. McQueen, and N. P. Armitage. Anomalous three-dimensional bulk ac conduction within the Kondo gap of SmB6 single crystals . 2016. *Physical Review B*. **94** (16): 165154.

Advancing Mesoscale Imaging for Dynamic Experiments at Current and Future X-ray Light Sources

Richard Sandberg
20170637ER

Project Description

The possibility of improving the majority of our current technological capabilities is limited by material properties. There is a demand for intelligent design of materials with tailored properties across many industries and applications; for example, high-strength steels for the automotive industry, damage resistant lightweight metals for military applications, and corrosion/temperature tolerant materials for the energy industry. In order to design these smart materials, we must understand the relationship between strain accumulation in a microstructure and the ensuing damage, which eventually leads to failure. This project aimed to advance mesoscale dynamic imaging by analyzing the theoretical requirements and current experimental limitations of multiple grain Bragg coherent diffraction imaging (BCDI) as a means to obtain 3D mesoscale characterization of polycrystalline samples. Developing this ability to map multiple grains with BCDI will provide nanometer scale grain distribution, orientation, and strain mapping in order to provide a 'pre-shot' analysis of a sample that will subsequently be dynamically loaded.

Technical Outcomes

Through this project we imaged (50nm resolution) the dislocation of a single copper grain in a metal film under tensile loading. We conducted experiments to observe the time evolution of strain as we pulled on the metal film. This work – the first such BCDI measurement in a free-standing film - has been submitted to Nature Communications. Additionally, our work has been presented as part of two invited talks.

Publications

Sandberg, R. L., and S. Fensin. Revolutions in Coherent X-ray Sources Will Enable Dynamic Nanometer Scale Strain Imaging in Structural Materials. Presented at *Materials Science and Technology*.(Salt Lake City, 25 October 2016).

Sandberg, R. L. Seeing damage and failure in structural materials at the ATOMIC scale. Presented at *ATOMIC APS-U Workshop*.(Lemont Illinois, 1 May 2017).

Three-dimensional X-ray diffraction imaging of dislocations in polycrystalline metals under tensile loading . Submitted to *Nature Communications*.



Nuclear and Particle Futures

Studying Nuclear Astrophysics and Inertial Fusion with Gamma-rays

Alex Zylstra
20150717PRD2

Project Description

The proposed work has two parts: studying nuclear astrophysics and basic nuclear physics, and developing a unique burning-plasma diagnostic capability for inertial confinement fusion (ICF) implosions. The field of nuclear astrophysics will benefit from high-quality measurements at low energies; the direct applicability of ICF plasmas to conditions in the universe is a unique opportunity to make substantial contributions to our understanding of stellar and big-bang nucleosynthesis. Basic nuclear physics of these few-nucleon systems will be simultaneously studied. This project will result in improved nuclear diagnostics for experiments at National Ignition Facility, which are important for achieving our goal of fusion ignition, in support of stockpile stewardship and fusion energy applications.

Publications

Rosenberg, M. J., F. H. Seguin, P. A. Amendt, Atzeni, H. G.

Rinderknecht, N. M. Hoffman, A. B. Zylstra, C. K. Li, Sio, M. G. Johnson, J. A. Frenje, R. D. Petrasso, V. Y. Glebov, Stoeckl, Seka, F. J. Marshall, J. A. Delettrez, T. C. Sangster, Betti, S. C. Wilks, Pino, Kagan, Molvig, and Nikroo.

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A B Zylstra, J A Frenje, P E Grabowski, C K Li, G W Collins, P Fitzsimmons, S Glenzer, F Graziani, S B Hansen, S X Hu, M Gatu Johnson, P Keiter, H Reynolds, J R Rygg, F H Séguin, and R D Petrasso. Development of a WDM platform for charged-particle stopping experiments. 2016. *Journal of Physics: Conference Series*. **717** (1): 012118. <http://stacks.iop.org/1742-6596/717/i=1/a=012118>.

Zylstra, A. B., H. W. Herrmann, M. G. Johnson, Y. H. Kim, J. A. Frenje, G. Hale, C. K. Li, M. Rubery, M. Paris, A. Bacher, C. R. Brune, C. Forrest, V. Y. Glebov, R. Janezic, D. McNabb, A. Nikroo, J. Pino, T. C. Sangster, F. H. S'eguin, W. Seka, H. Sio, C. Stoeckl, and R. D. Petrasso. Using Inertial Fusion Implosions to Measure the $T+3\text{He}$ Fusion Cross Section at Nucleosynthesis-Relevant Energies. 2016. *Phys. Rev. Lett.* **117**: 035002. <http://link.aps.org/doi/10.1103/PhysRevLett.117.035002>.

Zylstra, A. B., J. A. Frenje, P. E. Grabowski, C. K. Li, G. W. Collins, Fitzsimmons, Glenzer, Graziani, S. B. Hansen, S. X. Hu, M. G. Johnson, Keiter, Reynolds, J. R. Rygg, F. H. Seguin, and R. D. Petrasso. Measurement of Charged-Particle Stopping in Warm Dense Plasma. 2015. *PHYSICAL REVIEW LETTERS*. **114** (21).

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Nuclear and Particle Futures

Postdoctoral Research & Development
Continuing Project

Measurement of (n,g) Cross Sections Crucial for Constraining Stellar Nucleosynthesis

Aaron Couture
20170687PRD3

Project Description

The primary goal of this project is to determine the underlying reactions between the isotopes in stars. This determines the elements we find when we look out into the cosmos, as well as here on earth. In particular, elements heavier than iron have been made by neutrons in stars and stellar explosions. Understanding those reactions tells us about those stars and the cosmos. Many of the most informative reactions take place on unstable isotopes, making laboratory measurements even more challenging. In a similar way to the stellar archeology that tells us about the cosmos through telescopes and satellites, we can use the residue from man-made nuclear explosions to infer information about the yield and design of the device. These capabilities are a core component in DOE/NNSA mission for both Science-Based Stockpile Stewardship and Technical Nuclear Forensics missions. Again, many of the most discriminating reactions take place on unstable isotopes. The measurements performed as part of this project will develop techniques that can then be used to answer these national security questions.

Using X-Rays with Protons for a Material-Identification Capability via Proton Radiography

Levi Neukirch
20160652PRD2

Project Description

A single source of x-rays produces a wide range of energies, which often degrades the quality of an x-ray image. We will exploit this characteristic of x-ray sources to make simultaneous images from different energies in the x-rays spectrum. The attenuation of x-rays of different energies can be used to identify the materials present, so the images can be combined to make a 2D map of materials. The images can be fast enough to capture the details of plumes, jets, and ejecta produced in explosively driven systems. We will then further combine x-radiography with proton radiography for an even more sensitive pixel-by-pixel material identification diagnostic of dynamic systems. This technique will help answer very important questions about materials transport in shock physics experiments, such as what are the constituents of gas plumes and ejecta, and tell us where these constituents originated. Even a proof-of-principle demonstration of the technique with a static manufactured model will produce a high-impact publication of an important novel diagnostic.

Publications

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- Matthew Stouten Freeman. , Jason Clark Allison, John Jerome III Goett, Julian Daniel Lopez, Fesseha Gebre Mariam, Michael J. Martinez, Jason Jerry Medina, Frank Edward Merrill, Christopher Morris, Levi Patrick Neukirch, Abel John Raymer, Alexander Saunders, Tamsen Schurman, Amy Marie Tainter, Zhaowen Tang, Frans Raymond Trouw, Dale Tupa, Joshua L. Tybo, Wendy Vogan McNeil, and Carl Huerstel Wilde. Proton Radiography as a High Explosive Diagnostic Tool. 2017. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-30662>.
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A Rigorous Multiscale Method to Couple Kinetic and Fluid Models

Xianzhu Tang
20160361ER

Project Description

We will develop a rigorous multiscale method that couples kinetic (microscopic) model at internal boundary layers to a global continuum (macroscopic) model elsewhere for superior computational efficiency and global physics fidelity. This project will produce a physically sound and mathematically rigorous multiscale scheme that couples a non-perturbative kinetic model at internal boundary layers (IBL) to a perturbative fluid model away from the IBLs. We will demonstrate the fidelity and efficiency of the multiscale scheme in two prototypical applications of importance to space weather, inertial confinement fusion, and magnetic confinement fusion. DOE has identified these problems as key mission challenges in national security and energy security. Our innovation is also of a fundamental nature in the context of kinetic transport theory and multiscale modeling.

Publications

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The Cosmogenic Origins of ^{60}Fe

Aaron Couture
20160173ER

Project Description

In this project, we will perform measurements taking advantage of beams of iron-59 to study the nuclear physics needed to provide robust reaction rate predictions and incorporate them into hydrodynamic models of the supernova progenitor. The successful completion of this project will deliver, for the first time, experimentally based iron-60 yield and uncertainties from a core-collapse supernova. It will provide first studies of turbulence-based asymmetries in that yield. In the process of answering this over-arching question, it will answer additional questions about anomalous low-lying strength in the photon-strength function of iron isotopes, including answering questions about the multipolarity of that strength. This project will test and implement techniques to provide reliable neutron capture cross sections in regions where they cannot be measured directly, a critical step towards developing a fully predictive theoretical framework for nuclear reaction cross-sections in intermediate and heavy nuclei.

Publications

Liddick, S. N., Spyrou, B. P. Crider, Naqvi, A. C. Larsen, Guttormsen, Mumpower, Surman, Perdikakis, D. L. Bleuel, Couture, L. C. Campo, A. C. Dombos, Lewis, Mosby, Nikas, C. J. Prokop, Renstrom, Rubio, Siem, and S. J. Quinn. Experimental Neutron Capture Rate Constraint Far from Stability. 2016. *PHYSICAL REVIEW LETTERS*. **116** (24).

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Kinetic Modeling of Next-Generation High-Energy High-Intensity Laser-Ion Accelerators as an Enabling Capability

Lin Yin
20160472ER

Project Description

This project will apply a best-in-class vector particle-in-cell (VPIC) kinetic modeling capability on Los Alamos supercomputing platforms to guide a comprehensive, theoretical study of nonlinear, relativistic, laser-plasma interaction physics. Laser-driven ion accelerators enable important applications in high energy density science, matter in the extremes, and diagnostic science at the Laboratory. Such short pulse lasers continue to be a vital development path for advanced diagnostics of materials, and our work will help define more clearly the design requirements of facilities like MaRIE. The culmination of this work will be an advanced, validated design capability for developing ion sources of relevance to Los Alamos science campaigns.

Publications

Albright, B. J., L. Yin, and A. Favalli. Neutron generation from laser-accelerated ion beams: use of alternative deuterium-rich targets for improved neutron yield and control of neutron spectra. Submitted to *LASER and PARTICLE BEAMS*.

Stark, D. J., L. Yin, B. J. Albright, and F. Guo. Effects of dimensionality on kinetic simulations of laser-ion acceleration in the transparency regime. 2017. *PHYSICS of PLASMAS* . **24**: 056702.

Bridging Knowledge Gaps in Simulations of ICF Implosions

Andrei Simakov
20160458ER

Project Description

Standard numerical simulation tools for Inertial Confinement Fusion miss some important physics and are thus not predictive. We will use our new code to identify which missing physics is important and assess how to include it into the standard codes. We hope to achieve four major goals: (i) to perform detailed kinetic studies of several individual physical mechanisms not included in hydrodynamic codes and assess their importance; (ii) to carry out several integrated kinetic simulations of realistic implosions of gas-filled OMEGA capsules and, by comparing with hydrodynamic simulations, assess which kinetic mechanisms play important roles under realistic circumstances; (iii) this should allow us to start charting applicability boundaries for hydrodynamic simulations of gas-filled capsule implosions; (iv) once the importance of a kinetic mechanism is established, we will explore possible approaches for incorporating the missing physics into hydrodynamic codes.

Publications

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Taitano, W., L. Chacon, A. N. Simakov, and B. Keenan. Preliminary Simulations of Problems Related to ICF, and Verification Study with iFP. Presented at *Kinetic Physics in ICF Workshop 2016*. (LLNL, Livermore, CA, 5-7 Apr. 2016). <http://https://lasers.llnl.gov/nif-workshops/kinetic-physics-workshop-2016>.

Simakov, A. N., B. D. Keenan, W. T. Taitano, and Chacon. Plasma ion stratification by weak planar shocks. 2017. *PHYSICS OF PLASMAS*. **24** (9).

Shining Light on the Dense Gluon Structure of Large Nuclei

Ivan Vitev
20160183ER

Project Description

We will perform the first global extraction of a new class of 3D gluon densities in heavy nuclei, make them available to the wider community, and establish conclusively if a quantum coherent scattering regime has been reached in proton-nucleus reactions. Nucleons (protons and neutrons) are not fundamental building blocks of matter, but are in turn made up of quarks and gluons. Quantum Chromodynamics (QCD), the underlying theory of strong interactions, describes how quarks and gluons determine the properties of nucleons and nuclei. The overarching goal of this project is to develop theoretical and computational tools to unambiguously identify and accurately characterize such novel quantum coherent scattering regime of QCD at the Relativistic Heavy Ion Collider and the Large Hadron Collider. This work will enhance national scientific capabilities needed to address DOE milestones set by the Nuclear Science Advisory committee.

Publications

Vitev, I. Initial-state in-medium mremstrahlung contribution to soft and hard processes in reactions with nuclei . Presented at *Emerging Spin and Transverse Momentum Effects in p+p and p+A Collisions*.(Upton, NY, Feb. 8-10 2016).

Ringer, F. The jet fragmentation function in pp and ep collisions. Presented at *Joint CTEQ Meeting and POETIC 7*. (Philadelphia, PA, Nov. 14 – 18 2016).

Vitev, I. Opportunities with jet physics in e+A collisions. Presented at *POETIC7 and CTEQ Joint Meeting*. (Philadelphia, PA, Nov. 14 – 18 2016).

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Sievert, M. Contribution of small-x quark polarization to the proton spin. Presented at *RIKEN BNL Research Center Workshop: Saturation: Recent Developments, New Ideas and Measurements*.(Upton, NY, April 25 -27, 2017).

Sievert, M. Small-x asymptotics of the quark helicity distribution. Presented at *POETIC 2016*.(Philadelphia, PA, Nov. 14 – 18 2016).

Vitev, I. Jets and nuclear modifications at EIC . Presented at *Next Generation Nuclear Physics with JLab12 and EIC* . (Miami, FL, Feb. 10 – 13 2016).

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Vitev, I. Application SCET with Glauber gluons to heavy ion observables at NLO. Presented at *SCET 2017*.(Detroit, MI, Mar. 14-16, 2017).

Ovanesyan, , Ringer, and Vitev. Initial-state splitting kernels in cold nuclear matter. 2016. *PHYSICS LETTERS B*. **760**: 706-712.

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Next Generation Radiation Hydrodynamics for Astrophysics

Joshua Dolence
20170527ECR

Project Description

A variety of national security challenges require the use of sophisticated multi-physics simulations. The codes used for these simulations must be robust for a diverse set of applications, run efficiently on ever changing hardware, and produce accurate results to enable fruitful insights into the behavior of complicated systems. Radiation transport and coupling to matter has traditionally been one of the most challenging aspects in developing these multi-physics simulation codes. This project will serve to generalize a novel approach for treating radiation, targeting long-standing and fundamental problems in astrophysics: core-collapse supernovae and black hole accretion. These applications, aside from their intrinsic interest in the astrophysics community, have radiation physics as a central player and span a wide range of conditions. The outcomes of this project will include the most sophisticated and accurate simulations of both core-collapse supernovae and black hole accretion performed in the several decades over which modeling efforts have been conducted. In the process, the radiation transport method will have been refined and hardened, preparing it for use in other challenging areas such as those faced in national security applications.

Publications

- Radice, D., A. Burrows, D. Vartanyan, M. A. Skinner, and J. C. Dolence. Electron-capture and low-mass iron-core-collapse supernovae: new neutrino-radiation-hydrodynamics simulations. To appear in *Astrophysical Journal*.
- Ryan, B. R., S. M. Ressler, J. C. Dolence, A. Tchekhovskoy, C. Gammie, and E. Quataert. The Radiative Efficiency and Spectra of Slowly Accreting Black Holes from Two-temperature GRRMHD Simulations. 2017. *Astrophysical Journal Letters*. **844**: L24.
- Richers, S., H. Nagakura, C. D. Ott, J. Dolence, K. Sumiyoshi, and S. Yamada. A Detailed Comparison of Multidimensional Boltzmann Neutrino Transport Methods in Core-collapse Supernovae. 2017. *Astrophysical Journal*. **847**: 133.

Turbulence in Supernova Progenitors

Christopher Fryer
20160681PRD4

Project Description

Convection and turbulence are important factors in a wide number of problems, both for academic studies (e.g. supernovae, stars) and core DOE problems of direct national importance (from coal burning to problems in the national ignition facility). This post-doctoral effort seeks to build a bridge between scientists studying the academic problems and scientists working problems of direct national interest. Until recently, groups performing turbulence experiments, code developers at Los Alamos, and code developers in academia have worked separately. The lack of communication between these groups has hampered progress. The postdoc fellow funded through this project will work with all these groups to study convection and turbulence. As he progresses, he will tighten his ties within Los Alamos programs, and at the same time, apply his new knowledge to the academic problem of stellar convection, thereby strengthening collaboration between the Laboratory and the broader scientific community.

Publications

Jones, , F. K. Roepke, Pakmor, I. R. Seitenzahl, S. T. Ohlmann, and P. V. F. Edelmann. Do electron-capture supernovae make neutron stars? First multidimensional hydrodynamic simulations of the oxygen deflagration. 2016. *ASTRONOMY & ASTROPHYSICS*. **593**.

Precision Theoretical Analysis of Reactions with Protons Polarized in a Strong Magnetic Field

Ivan Vitev
20160645PRD1

Project Description

This project will allow much-improved understanding of the internal structure of protons and neutrons. It will extend the applicability of the theory of strong interactions to reactions with particles polarized by strong magnetic fields. Precision analysis of measurements from the polarized proton experiment at Fermilab will help construct a 3D picture and contribute to the resolution of the longstanding problem about the origin of the nucleon spin. This work addresses DOE's vision for the future of nuclear physics, as well as priorities set for DOE to study the internal structure of nucleons.

Publications

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- Ishikawa, T., Y. Q. Ma, J. W. Qiu, and S. Yoshida. Matching issue in quasi parton distribution approach. 2017. In *34th International Symposium on Lattice Field Theory*. (Southampton, 24-30 July 2016). p. 177. Southampton: Proceedings of Science. <http://https://pos.sissa.it/256/>.
- Ishikawa, T., Y. Q. Ma, J. W. Qiu, and S. Yoshida. On the renormalizability of quasi parton distribution functions. To appear in *Physical Review D*. <http://https://arxiv.org/abs/1707.03107>.
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- Koike, Y., A. Metz, D. Pitonyak, K. Yabe, and S. Yoshida. Twist-3 fragmentation contribution to polarized hyperon production in unpolarized hadronic collisions. 2017. *Physical Review D*. **95** (11): 114013. <http://https://journals.aps.org/prd/abstract/10.1103/PhysRevD.95.114013>.
- Hatta, Y., B. Xiao, S. Yoshida, and F. Yuan. Single spin asymmetry in forward pA collisions II: Fragmentation contribution. 2017. *Physical Review D*. **95** (1): 014008. <http://https://journals.aps.org/prd/abstract/10.1103/PhysRevD.95.014008>.
- Gamberg, L., Z. B. Kang, M. Schlegel, H. Xing, and S. Yoshida. Evolution equations for the collinear twist-3 functions related to the transverse momentum weighted TMD functions. Presented at *QCD Evolution 2017*. (Virginia, 22-26 May 2017).
- Ishikawa, T., Y. Q. Ma, J. W. Qiu, and S. Yoshida. Practical quasi parton distribution functions. To appear in *Physical Review D*. <http://https://arxiv.org/abs/1609.02018>.
- Gamberg, L., Z. B. Kang, M. Schlegel, H. Xing, and S. Yoshida. Scale evolution equations for transverse momentum weighted TMD functions. Presented at *7th Workshop of the APS Topical Group on Hadronic Physics*. (Washington, DC, 1-3 Feb. 2017).

Nuclear and Particle Futures

Directed Research
Continuing Project

Rapid Response to Future Threats (U)

Charles Nakhleh
20160664DR

Project Description

This project addresses weapons design challenges for the 21st century by laying the groundwork that enables weapons designers to respond quickly and efficiently to mission needs. At its end, this project will supply the first version of a set of tools that will enable a designer to quickly and efficiently execute design iteration calculation with modern design codes. The project will also provide the calculational modeling for developing a non-traditional weapons physics package outside the design space of the existing stockpile.

Dark Matter Search with a Neutrino Experiment

Richard Van De Water
20160037DR

Project Description

The project will significantly improve the search for sub-GeV Dark Matter with the Short Baseline Neutrino Detector (SBND) at Fermilab by building a powerful photon detection system, and developing new theoretical models of the Dark Sector physics. Final state charged particles that interact in the SBND liquid argon time projection chamber produce recoil electrons, which in turn produce scintillation light that can be detected by the photon detection system (PDS). The PDS reconstructs the neutrino or dark matter event position and time from the scintillation light. The timing of the scintillation light is approximately one nanosecond, which enables the PDS to significantly reduce backgrounds and expand the physics scope of SBND by enabling a search for sub-GeV dark matter. The development of liquid argon scintillation light detection capability at Los Alamos could lead to applications in nuclear nonproliferation such as enhanced neutron and gamma-ray portal detection.

Publications

Van de Water, R. G. SBND PMT System Review. 6. *Fermi National Accelerator Laboratory Systems Review Nov 18, 2016* .

Battaglieri, M., and others. US Cosmic Visions: New Ideas in Dark Matter 2017: Community Report. 2017.

Nuclear and Particle Futures

Exploratory Research
Continuing Project

Lepton Number Violation: Connecting the Tera Electron Volt (TeV) Scale to Nuclei

Vincenzo Cirigliano
20170290ER

Project Description

Neutrinoless double beta decay is a rare nuclear process whose observation would prove that neutrinos, the most elusive elementary particles, coincide with their own antiparticles. This could happen only if at a fundamental level the "matter number" is not conserved in nature. The observation of such a process would therefore have deep implications on our understanding of the matter-antimatter asymmetry in the universe. In the Nuclear Science Advisory Committee's 2015 Long Range Plan, the US Nuclear Physics community identified "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 developing a broader theoretical framework for the interpretation of neutrinoless double beta decay searches, our project will strengthen the case for such a high-profile DOE endeavor.

Publications

- Cirigliano, V., W. Dekens, J. de Vries, M. Graesser, and E. Mereghetti. Neutrinoless double beta decay in chiral effective field theory: lepton number violation at dimension seven. Submitted to *Journal of High Energy Physics*. <http://https://arxiv.org/abs/1708.09390>.
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Nuclear and Particle Futures

Exploratory Research
Continuing Project

Realization of a Laboratory Turbulent Magnetic Dynamo: A Gateway to New Laboratory Astrophysics and Inertial Confinement Fusion Experiments

Kirk Flippo
20170367ER

Project Description

When plasmas flow they create electric and magnetic fields, and as it turns out, these processes essentially magnetize the entire universe; turbulent magnetic dynamo in particular is poorly understood. Recently it has been suggested that these fields can also have a larger impact on the flow of plasmas on the small scale, like in an Inertial Confinement Fusion (ICF) capsule, than previously had been thought. This could lead to degradation in ICF yields. This project will help us understand how easily and how strongly these fields are created under similar conditions using a turbulent plasma plume design. Studying how these dynamos can saturate is an important step in understanding how important these fields can be to the dynamics of an ICF implosion.

Publications

Flippo, K. A., A. Rasmus, H. Li, S. Li, T. Cardenas, C. Kuranz, J. Levesque, S. Klein, and P. Tzeferacos. Towards a turbulent magnetic dynamo platform. 2017. In *Bulletin of the American Physical Society 59th Division of Plasma Physics Conference*. (Milwaukee, Oct 23-27, 2017). p. 1. Los Alamos: LANL.

Nuclear and Particle Futures

Early Career Research
Continuing Project

Laser-Based Mega Electron Volt (MeV) X-ray Source for Double-Shell Radiography

Sasikumar Palaniyappan
20170573ECR

Project Description

Imaging dense materials requires Mega electron volt x-rays. Traditionally such x-rays are generated by impinging mega electron volt electrons from linear accelerators onto high-Z material such as tungsten or tantalum. However, these linear accelerators are very expensive and large in size. Several applications, such as imaging a NIF double shell implosion, require a compact mega electron volt x-ray source. This project aims to develop such a compact x-ray source by generating an energetic electron beam using compact intense lasers and impinging those electrons onto a tantalum converter foil. Such a compact x-ray source is an essential tool for mega electron volt x-ray radiography.

Publications

- Fernandez, J. C., D. C. Gautier, Huang, Palaniyappan, B. J. Albright, Bang, Dyer, Favalli, J. F. Hunter, Mendez, Roth, Swinhoe, P. A. Bradley, Deppert, Espy, Falk, Guler, Hamilton, B. M. Hegelich, Henzlova, K. D. Ianakiev, Iliev, R. P. Johnson, Kleinschmidt, A. S. Losko, McCary, Mocko, R. O. Nelson, Roycroft, M. A. S. Cordoba, V. A. Schanz, Schaumann, D. W. Schmidt, Sefkow, Shimada, T. N. Taddeucci, Tebartz, S. C. Vogel, Vold, G. A. Wurden, and L. i. n. Yin. Laser-plasmas in the relativistic-transparency regime: Science and applications. 2017. *PHYSICS OF PLASMAS*. **24** (5).
- Tobias, B. J., S. Palaniyappan, D. C. Gautier, J. Mendez, T. Burris-Mog, C. K. Huang, A. Favalli, J. F. Hunter, M. E. Espy, D. W. Schmidt, R. O. Nelson, A. Sefkow, T. Shimada, R. P. Johnson, and J. C. Fernandez. Quantification of uncertainty in photon source spot size inference during laser-driven radiography experiments at TRIDENT. 2017. *LA-UR-17-28604*. <http://permalink.lanl.gov/object/view?what=info:lanl-repo/lareport/LA-UR-17-28604>.

Gluon Saturation Search with Large Hadron Collider Beauty (LHCb) Experiment

Cesar Da Silva
20170569ECR

Project Description

Gluons are one of the fundamental particles inside protons and neutrons; they are responsible for the strong nuclear force which hold nucleons inside nucleus. Gluon is a boson, which means it can merge in a condensate form, sharing the same energy level, if they are too close each other. This new form of gluon saturated nuclear matter is up to discovery and can explain many of the behaviors observed in particle and nuclear physics in high-energy collisions at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory and the Large Hadron Collider (LHC) at CERN. The LHCb experiment at LHC is the only experiment in the world which can access unexplored kinematic regions where gluon saturation is expected. This project aims to make the first search and detector prototype of a particle tracker inside the LHCb magnet to extend the experimental coverage in the expected gluon saturated region. The unambiguous discovery of gluon saturation and how nuclear matter behaves in this state will have several implication on particle production in high energy collisions, understanding of the sources of the strong nuclear forces, and can help describe the Universe a few microseconds after the Big-Bang.

Revealing the Particle Nature of Dark Matter with Cosmic Gamma Rays

Andrea Albert
20160641PRD2

Project Description

Most of the mass in the Universe is Dark Matter (DM) of an entirely unknown nature. A strong candidate for dark matter, based on high-energy physics theories, would produce high-energy gamma rays. This project will result in the most sensitive searches for gamma-ray signals from massive DM candidates. These searches will rule out some models of the DM if no signal is detected; however, if a signal is detected then other observations from the High Altitude Water Cherenkov Observatory and Fermi Large Area Telescope will have to be consistent with this signal. This would be a major discovery solving one of the longest standing problems in astrophysics, cosmology, and particle physics. The project also builds capabilities relevant to nuclear weapons research and nuclear nonproliferation through development and analysis of data from complex detectors.

Publications

Acero, , Ackermann, Ajello, Albert, W. B. Atwood, Axelsson, Baldini, Ballet, Barbiellini, Bastieri, Belfiore, Bellazzini, Bissaldi, R. D. Blandford, E. D. Bloom, J. R. Bogart, Bonino, Bottacini, Bregeon, R. J. Britto, Bruel, Buehler, T. H. Burnett, Buson, G. A. Caliandro, R. A. Cameron, Caputo, Caragiulo, P. A. Caraveo, J. M. Casandjian, Cavazzuti, Charles, R. C. G. Chaves, Chekhtman, C. C. Cheung, Chiang, Chiaro, Ciprini, Claus, Cohen-Tanugi, L. R. Cominsky, Conrad, Cutini, D'Ammando, de Angelis, DeKlotz, de Palma, Desiante, S. W. Digel, Di Venere, P. S. Drell, Dubois, Dumora, Favuzzi, S. J. Fegan, E. C. Ferrara, Finke, Franckowiak, Fukazawa, Funk, Fusco, Gargano, Gasparrini, Giebels, Giglietto, Giommi, Giordano, Giroletti, Glanzman, Godfrey, I. A. Grenier, M. -. Grondin, J. E. Grove, Guillemot, Guiriec, Hadasch, A. K. Harding, Hays, J. W. Hewitt, A. B. Hill, Horan, Iafate, Jogler, Johannesson, R. P. Johnson, A. S. Johnson, T. J. Johnson, W. N. Johnson, Kamae, Kataoka, Katsuta, Kuss, La Mura, Landriu, Larsson, Latronico, Lemoine-Goumard, Li, Li, Longo, Loparco, Lott, M. N. Lovellette, Lubrano, G. M. Madejski, Massaro, Mayer, M. N. Mazziotta, J. E. McEnery, P. F. Michelson, Mirabal, Mizuno, A. A. Moiseev, Mongelli, M. E. Monzani, Morselli, I. V. Moskalenko, Murgia, Nuss, Ohno, Ohsugi, Omodei, Orienti, Orlando, J. F. Ormes, Paneque, J. H. Panetta, J. S. Perkins, Pesce-Rollins, Piron, Pivato, T. A.

Porter, J. L. Racusin, Rando, Razzano, Razzaque, Reimer, Reimer, Reposeur, L. S. Rochester, R. W. Romani, Salvetti, Sanchez-Conde, P. M. S. Parkinson, Schulz, E. J. Siskind, D. A. Smith, Spada, Spandre, Spinelli, T. E. Stephens, A. W. Strong, D. J. Suson, Takahashi, Takahashi, Tanaka, J. G. Thayer, J. B. Thayer, D. J. Thompson, Tibaldo, Tibolla, D. F. Torres, Torresi, Tosti, Troja, Van Klaveren, Vianello, B. L. Winer, K. S. Wood, Wood, and Zimmer. FERMILARGE AREA TELESCOPE THIRD SOURCE CATALOG. 2015. *ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES*. **218** (2).

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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.

Publications

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Enabling Electron Excitations in the Modeling of Warm Dense Matter

Jerome Daligault
20170490ER

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 tools we are developing in this project will open the door to simulations of non-equilibrium processes in WDM. This will greatly advance our ability to compute self-consistently a large number of physical properties of WDM. In particular, programmatically relevant processes include the energy exchange rates between electrons and ions, and the stopping power of charged projectiles.

Publications

Daligault. Crossover from Classical to Fermi Liquid Behavior in Dense Plasmas. 2017. *PHYSICAL REVIEW LETTERS*. **119** (4).

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Nuclear and Particle Futures

Exploratory Research
Continuing Project

Beat-Wave Magnetization of a Dense Plasma

Scott Hsu
20170457ER

Project Description

The beat-wave magnetization problem studied in this project could enable a new lower-cost pathway to fusion energy, synergistic with the approaches being studied as part of the ARPA-E ALPHA program in developing lower-cost approaches to fusion energy.

New Science and Technology for a Tabletop Accelerator.

Evgenya Simakov
20170006DR

Project Description

The project will deliver a stand-alone laser powered compact accelerator that produces mega-electron-volt electron beams with femtosecond bunch lengths. Dielectric laser accelerator (DLA) technology has been identified as one of the most promising advanced accelerator approaches by both the accelerator community and the Office of Science/High Energy Physics (HEP) directorate, and is arguably the best match for compact light sources and accelerators for medical therapy and national security. Compact accelerators are desired by a number of national security applications, including war-fighter support (weaponized FELs) and active interrogation (electron accelerators as compact front ends for muon active interrogation sources or to generate bremsstrahlung radiation). With increased efficiency and decreased weight provided by DLA technology FELs might become fieldable on airborne platforms. This work also positions Los Alamos at the forefront of advanced high current cathode development for multi-megawatt accelerators for applications such as environmental remediation (e.g., cleaning up toxic chemical spills), and accelerator-driven fission power.

Publications

Andrews, H. L., R. L. Fleming, J. W. Lewellen, K. E. Nichols, D. Y. Shchegolkov, E. I. Simakov, and B. K. Choi. Current Experimental Work with Diamond Field-Emitter Array Cathodes. To appear in *38th Free Electron Lasers Conference (FEL 2017)*.(Santa Fe, NM, August 20-25, 2017).

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Simakov, E. I., H. L. Andrews, M. J. Herman, K. M. Hubbard, and Weis. Diamond Field Emitter Array Cathodes and Possibilities of Employing Additive Manufacturing for Dielectric Laser Accelerating Structures. 2017. *ADVANCED ACCELERATOR CONCEPTS*. **1812**.

Quantum Effects on Cosmological Observables: Probing Physics Beyond the Standard Model

Mark Paris
20170430ER

Project Description

The Laboratory's mission to maintain the safety and reliability of the nuclear stockpile requires detailed numerical computations that describe how weapons function. In particular, ever-more precise and complete descriptions of the nuclear reactions, which our proposal will constrain to high accuracy, are required. This project will use new, precision data obtained from astronomy and cosmology from some of the largest observables length scales to constrain the microscopic physics relevant for nuclear reactions, which are also important for understanding the function of nuclear weapons.

Publications

Johns, L., M. Mina, V. Cirigliano, M. W. Paris, and G. M. Fuller. Neutrino flavor transformation in the lepton-asymmetric universe. 2016. *Phys. Rev.* **D94** (8): 083505.

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Cirigliano, V., M. W. Paris, and S. Shalgar. Effect of collisions on neutrino flavor inhomogeneity in a dense neutrino gas. 2017. *Physics Letters B*.

Understanding Ejecta, Transport, Break-up and Conversion Processes (U)

William Buttler
20170082DR

Project Description

The scientific understanding essential for stockpile stewardship encompasses a broad range of phenomena that require a concerted effort in theoretical and experimental physics. The phenomena occurring at high density and very short micro-second time scales require sophisticated, frontier, experimental techniques and new theoretical methods. These are joined in this project for one of the unresolved issues in the physics of what occurs when a shockwave impacts a metal-gas interface susceptible to chemical reaction, in this case hydriding at a cerium-hydrogen gas interface. The detailed understanding of the state, composition, size and velocity of hydride material particulates (ejecta) produced that this project will provide will result in essential understanding and predictive models for these important phenomena for the first time.

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Schauer, M. M., W. T. Buttler, D. S. Sorenson, D. K. Frayer, M. Grover, B. M. LaLone, G. D. Stevens, and W. D. Turley. Constraining ejecta particle size distributions with light scattering. To appear in *20th Biennial International Conference of the APS Topical Group on Shock Compression of Condensed Matter*. (St. Louis, Missouri, 9-14 July 2017).

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Probing Quark-Gluon Plasma with Bottom Quark Jets at sPHENIX

Ming Liu
20170073DR

Project Description

The goal of this project is to address important physics questions in Quark-Gluon-Plasma (QGP) physics using the sPHENIX experiment at the Relativistic Heavy Ion Collider at the Brookhaven National Lab. Measurements of modification of heavy quark production in high energy heavy ion collisions at RHIC will help us to understand various quark energy loss mechanisms, including radiative and collisional energy loss inside QGP. This project will allow us to develop a new heavy quark physics program for the next generation heavy ion detector, sPHENIX.

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Dark Matter and the Validity of Effective Field Theories

Michael Graesser
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.

Nuclear and Particle Futures

Postdoctoral Research & Development
Continuing Project

Jets in Strongly Interacting Plasmas

Ivan Vitev
20170666PRD1

Project Description

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 CERN. An extremely dense and hot “fireball” is created in collisions of heavy ions and consists of the elementary constituents of matter, quarks 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

Publications

Brewer, J., K. Rajagopal, A. Sadofyev, and W. van der Schee.
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Distribution of an Ensemble of Holographic Jets in Strongly
Coupled Plasma. Submitted to *Journal of High Energy
Physics*. <http://https://arxiv.org/abs/1710.03237>.

Search for Low Mass Dark Photons in High Energy Proton-Nucleus (p+A) Collisions at Fermilab

Ming Liu
20160081ER

Project Description

A new detector and theory will be developed in this project to identify the signal of dimuons from dark photon decays at Fermilab. Dark photons are a candidate for dark matter that is needed to account for the key properties of the observed Universe. We propose to carry out a new direct search for dark photons by colliding the 120GeV proton beam from the Fermilab Main Injector with the 5m thick iron beam dump at the E906 experiment. With the world highest integrated luminosity, we could directly create and detect dark photons in the so called visible decay mode. A new dedicated trigger detector will be developed in this project to identify dimuon events from dark photon decays. The development of new fast high-resolution tracking detectors and trigger systems would benefit global security and the production of materials at the mesoscale.

Publications

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- Liu, M., K. Liu, and S. Uemura. Dark Sectors 2016 Workshop: Community Report. 2016. *Dark Sectors 2016 Workshop*. <http://arxiv.org/abs/1608.08632>.
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Cosmic Positrons from Pulsar Winds and Dark Matter

Brenda Dingus
20160007DR

Project Description

Satellite observations reveal a puzzling excess of cosmic positrons, the anti-matter partner of electrons. We will use observations of high energy gamma rays and theoretical models to constrain positrons from astrophysical sources and from dark matter. While the existence of dark matter is well known, the nature of the particles that comprise dark matter is not. With this project, we will increase our understanding of the possible properties of dark matter. Also, the existence of high energy emission from pulsars is well known; however, the physical mechanisms by which the particles are accelerated is not. With this project, we will detect higher energies from pulsars and compare these observations with new theoretical models. Finally, we will use radiation transport simulations to predict the locally-measured, cosmic positrons from both dark matter and pulsars. These investigations will increase the Laboratory's capabilities in information science and technology as well as remote sensing of radiation and other experimental techniques relevant to studies of our nuclear stockpile.

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Adaptive Feedback for Automatic Phase Space Tuning of Electron Beams in Advanced X-ray Free-Electron Lasers

Alexander Scheinker
20170630ER

Project Description

Collaboration with Stanford Linear Accelerator Center and testing algorithms at Linac Coherent Light Source increases the Laboratory's core capability of advanced accelerator and controls algorithm development. By improving the performance of the light source, Los Alamos will see a direct benefit to our on-going weapons related experiments there. As the algorithms are, by design, model-independent and applicable to a wide range of complex systems, they will be of interest to other laboratories and industry that rely on accelerators. This work has the potential to improve the performance of existing particle accelerators and enable performance goals of future light sources such as the European X-ray Free Electron Laser and Matter and Radiation Interaction in Extremes.

Publications

Scheinker, A. Automatic Tuning and Control for Advanced Light Sources. To appear in *Materials Discovery and Design: Data Science and Optimal Learning*. Edited by Lookman, T., S. Eidenbenz, F. Alexander, and C. Barnes, Editors.

Scheinker, A., and D. Bohler. Adaptive Feedback for Automatic Phase-space Tuning of Electron Beams in Advanced XFELs. To appear in *International Free-Electron Laser Conference FEL 2017*.(Santa Fe, NM, 20-25 Aug. 2017).

Demonstration of Electron Beam Generation with a Novel Solid-State Amplifier Driven Accelerator for Space Deployment Applications

Dinh Nguyen
20170521ER

Project Description

Novel low-voltage-transistor-driven electron accelerators are needed for miniature, lightweight particle accelerators, which could enable cutting-edge tools for space science, environmental remediation, and homeland security missions. By eliminating high-power, high-voltage tube-based RF sources, the new accelerators will be less expensive, require less supporting infrastructure, and be safer to maintain and operate. The goal of this effort is to demonstrate the ability of a new class of RF amplifier chips, high-electron-mobility transistors (HEMTs), to successfully power a particle accelerator. Specifically, the research team has delivered an energy boost to electrons emitted from a commercial electron beam source, using an RF accelerator cavity driven by a single HEMT chip. Over a distance of approximately $1\lambda^2$ (6mm), electrons in the beam had been given a 15-kV increase in energy. This demonstration of energy gain in RF cavities individually driven by low-voltage transistors advances the readiness level of compact, lightweight RF accelerator technology, and demonstrates the promise of this technology to revolutionize the design, engineering and utilization of particle accelerators.

Publications

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Exploring the Multi-scale Physics that Regulates Black Hole Accretion

Joseph Smidt
20170317ER

Project Description

This project aims to provide the first definitive simulations showing how black holes with over a billion solar masses formed in the early universe. These calculations will require next-generation radiation-hydrodynamics simulations at many lengths scales. Understanding radiation hydrodynamics and radiation-matter coupling are primary science objectives of the Department of Energy (DOE). Black holes provide radiation feedback to matter on energy scales that range from a few eV to several keV. These radiation-hydrodynamical simulations will utilize multigroup radiation transport methods to analyze these feedback effects on matter that builds the underlying science of interest to the DOE. The effects of this multigroup radiation transport and matter coupling will be documented in our publications. The observational signatures published by this work will be directly used by NASA surveys such as JWST to classify supermassive black holes, as well as surveys that collaborate with NASA efforts such as ALMA. Probing black holes is one of NASA's main science goals and objectives. How the billion solar mass supermassive black holes formed in the early universe is one of the outstanding questions in cosmology. By detailing comprehensively how such black holes formed, this work will have a major impact on the cosmology and astrophysics communities.

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Publications

Smidt, J., D. J. Whalen, J. L. Johnson, and H. Li. The Formation of the First Quasars in the Universe. To appear in *The Astrophysical Journal*. <http://adsabs.harvard.edu/abs/2017arXiv170300449S>.

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Nuclear and Particle Futures

Exploratory Research
Continuing Project

Wakefield Study for Superconducting Accelerator Cavities

Bruce Carlsten
20170628ER

Project Description

What is known as "long-range wakefields" can degrade electron beam quality when there are bursts of closely spaced electron bunches, especially for beams in superconducting accelerators. This has the potential to impact future accelerators needed for national security and discovery science missions, such as the X-ray free-electron laser proposed for MaRIE, as well as future Department of Energy Office of Science accelerators for Basic Energy Science light sources or High Energy Physics energy frontier research. The consequence could be some limitation in the pulse structure of the burst or, alternatively, indicate a different accelerator architecture such as short-pulse, normal-conducting accelerators. This is a fundamental accelerator research question with urgency to answer.

Investigating Properties of Quark-Gluon Plasma using Jets and Heavy Quark Production at RHIC

Michael McCumber
20140665PRD2

Project Description

This project aims to initiate a new set of detector systems (sPHENIX) designed specifically for high-energy jet measurement. We will focus on a new research area of heavy ion physics using particle jet production as a probe to study the properties of quark-gluon plasmas. Success will open up a new research direction for the Los Alamos nuclear physics program. This work is an example of how basic experimental nuclear science delivers people, expertise, and ideas to applied nuclear programs.

Technical Outcomes

Dr. McCumber spearheaded the LANL role on future measurements at the Relativistic Heavy Ion Collider while making significant contributions to on-going experiments. During his fellowship he expanded the science case for future heavy-flavor quark measurements, advanced charged particle tracking techniques in heavy ion collisions, and demonstrated the advantage of MAPS-based tracking technology for new measurements. Dr. McCumber has now converted into LANL scientific staff and is currently applying his skills within the weapons program.

Publications

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A Step toward Nuclear Reaction Studies for Applications at FRIB

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Project Description

There is a knowledge gap in our understanding of nuclear reaction rates, which has significant impact for both astrophysics and stockpile stewardship. This project seeks to validate an experimental method to close this gap. The project will directly measure the ^{96}Zr neutron capture cross section using the Detector for Advanced Neutron Capture Experiments (DANCE) at Los Alamos, and constrain a theoretical calculation of the cross section using indirect techniques with the Apollo instrument at Argonne National Laboratory. Furthermore, DANCE can make an independent measurement of the nuclear structure properties of ^{96}Zr and independently constrain theoretical calculations of the capture cross section. It is expected that these three independent measurements will result in a consistent cross section prediction.

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Technical Outcomes

We ran experiments on $^{96}\text{Zr}(n,g)$ and $^{96}\text{Zr}(d,p)$ and analyzed the resulting gamma-ray cascades. The data illustrate the break-down of statistical nuclear behavior in the limit of low level density and associated limitation of statistical approaches to predicting neutron capture rates.

Publications

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Extreme-Scale Kinetic Plasma Modeling of Turbulence and Mix Using VPIC

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20150751ER

Project Description

We will substantially modify the vector particle-in-cell (VPIC) code to enable efficient use of the Trinity supercomputer to enable and perform groundbreaking simulations of plasma-phase mix and turbulence. The ability to resolve outstanding problems associated with plasma-phase mix ties directly to outstanding problems in high energy density science of direct importance to nuclear weapons programs. At the culmination of this project, we will have made substantial progress toward resolving outstanding physics problems in plasma and high energy density science. Specifically, we will have revealed through large-scale calculations how dense plasmas mix with one another. We also will have advanced our understanding of the physics of magnetic reconnection and the acceleration of cosmic ray particles to very high energy. Another legacy of this project will be the development of our VPIC particle-in-cell kinetic plasma code for modern supercomputers such as Trinity and future multi-core platforms.

Technical Outcomes

VPIC is general-purpose, kinetic plasma modeling code that has been applied to and validated on a variety of problems. We applied VPIC to two open science problems central to our understanding of turbulence and mix in space and laboratory plasmas. Both problem areas were sized appropriately for Trinity Phase 2, and represent credible paths for follow-on program development at the conclusion of this project.

Publications

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Cold Cathodes for Next Generation Electron Accelerators: Methodologies for Radically Improving Performance and Robustness

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Project Description

The purpose of this project is to understand and control the rich effects of nanostructure in cold cathode materials to make parallel, transformational advances in the two critical performance areas of an electron source: lifetime and efficiency. We will develop and demonstrate 'designer' cold cathode electron sources with tunable parameters (bandgap, efficiency, optical absorption) that outperform present technologies in terms of efficiency and lifetime, where success in either of these is considered transformational. We introduce fundamentally new approaches to address decadal weaknesses in performance and enable cathode properties to be tuned or engineered for specific DOE missions and related applications. Improved cold cathodes with controllable parameters allow for higher performance, reduced complexity, reduced cost, and reduced system maintenance in almost every relevant application area. It is directly enabling for all accelerator-based approaches to remote detection of chemicals, pathogens, and nuclear materials. It would benefit accelerator-based solutions for management of nuclear waste as well as the production of critical medical radioisotopes.

Technical Outcomes

This project developed high performance electron sources by utilizing nanoscale material properties, such as electronic structure, band gap, and quantum confinement, as design parameters. First-ever demonstrations include: photoemission from quantum dots; enhanced efficiency and lifetime via 2D coatings; tunable band gap; and material-independent design methodology for enhancing Quantum Efficiency via wave-interference effects. Rational design of cathode materials is a new frontier which can scale to address the evolving needs of existing and future next-generation accelerators.

Publications

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Nuclear and Particle Futures

Postdoctoral Research & Development
Final Report

A Kinetic Theory Based Study of Type II Core-Collapse Supernovae

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20150741PRD3

Project Description

We will model the dynamics of core-collapse supernovae with a first-of-a-kind kinetic theory based algorithm. The algorithm is capable of resolving the system's macroscopic hydrodynamics and treats neutrino transport for all mean free paths identically and on equal footing with the nuclear matter. This first-of-a-kind kinetic theory based core-collapse supernova model capable of resolving the system's macroscopic hydrodynamics that treats neutrino transport for all mean free paths identically and on equal footing with the nuclear matter will enhance the Laboratory's ability to model these systems, making the work relevant to our national security mission.

Technical Outcomes

We developed a kinetic particle code to capture physical flows for small and large particle mean-free-paths. While we focused on core-collapse supernovae, the code could also be applied to Inertial Confinement Fusion (ICF) simulations, as both systems are shaped by hydrodynamic and non-equilibrium phenomena. We tested our code via fluid instability, gravitational collapse, and implosion simulations. There was excellent agreement with hydrodynamic simulations and analytic solutions - showing promise for future supernova and ICF studies.

Publications

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k_{effective}: First Measurement of a Nanosecond-Pulsed Neutron Diagnosed Subcritical Assembly

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Project Description

With this project, we aimed to develop a precision measurement technique to determine the neutron generation in a subcritical system with accuracy comparable to that of nuclear testing. Previous subcritical experiments have not had the diagnostic capability to infer nuclear generation. Our project involving Neutron Diagnosed Subcritical Experiments (NDSE) provides neutron generation, which is an extremely sensitive integral constraint on both the distribution and nuclear properties of materials. Our proposed NDSE capability would enable inference of neutron generation or, more precisely, "alpha," with the accuracy needed for weapons analysis.

Technical Outcomes

We proved a single-shot accuracy of better than 0.3% for the NDSE technique. using static nuclear targets at the Nevada Site. Our experiment included a Dense-Plasma-Focus (DPF) source, custom detectors, and carefully designed shielding. Our MCNP6 and LA-COMPASS magneto-hydrodynamic simulations were validated by our experimental results. Through our work, the laboratory and the nation have the opportunity of a new test facility for alpha reaction history, similar to traditional reaction diagnostics employed during full-scale testing.

Publications

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Assessing the Quantum Physics Impacts on Future X-ray Free-electron lasers

Mark Schmitt
20150508ER

Project Description

This project successfully developed a new quantum mechanical theory of x-ray free electron lasers (XFELs) that has placed Los Alamos at the forefront of understanding quantum effects in XFELs. Our quantum theory describes the interaction of relativistic electrons with x-ray radiation in the periodic magnetic field of an undulator using the same mathematical formalism as classical XFEL theory. This places classical and quantum treatments on the same footing and allows for a continuous transition from one regime to the other, thereby eliminating the disparate analytical approaches previously used. The quantum treatment of XFELs developed in this project provides a foundation for the performance assessment of FELs in the short wavelength X-ray regime. The results of this work indicate that quantum effects will not produce a significant degradation of the fundamental and harmonic emission of XFELs in the MaRIE parameter regime. This research has strengthened the technical validity of the MaRIE XFEL design while simultaneously increasing both the theoretical FEL expertise at Los Alamos and the technical stature of the Laboratory in the international XFEL community.

Technical Outcomes

A new quantum mechanical theory for x-ray free electron lasers (XFELs) has been developed. It describes the interaction of relativistic electrons with x-rays using the same mathematical formalism as classical XFEL theory, allowing for a continuous transition from one regime to the other and eliminating the disparate analytical approaches previously used. Results indicate that quantum effects will not produce a significant degradation of the fundamental and harmonic emission of XFELs in the MaRIE parameter regime.

Publications

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Enhancing the Long-Baseline Neutrino Experiment Oscillation Sensitivities with Neutron Measurements

Keith Rielage
20150577ER

Project Description

We deploy our large liquid argon time-projection chamber in the high-energy neutron beamline at Los Alamos and measure neutron interactions in the detector; results will be applied to neutrino energy reconstruction for long-baseline neutrino experiments. We will study neutron interactions on liquid argon in terms of their event signatures and use the results to test existing simulations of the interactions. We will then modify those simulations with our high-statistics dataset. Ultimately, we will produce an oscillation analysis approach for the Long-Baseline Neutrino Experiment that includes the impact of neutrons as well as a requirement to be sensitive to new physics. This analysis will create the near neutrino detector requirements essential for making optimal design choices.

Technical Outcomes

Neutron interactions were successfully measured for the first time in a liquid argon time-projection chamber using a well-understood neutron beam. These data will be used to benchmark simulations for the DUNE neutrino experiment, under construction at Fermilab and in South Dakota, designed to look to violation of charge conjugation and parity (CP) symmetry by comparing neutrino and anti-neutrino oscillations. Such observations would help explain the matter-antimatter asymmetry of the Universe, a key scientific question.

Publications

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Magnetic Rayleigh-Taylor Instability

Daniel Livescu
20150568ER

Project Description

The project aims to answer if magnetic fields can control or constrain the hydrodynamic instabilities and mix in the context of inertial confinement fusion. Our results will be valuable for fusion experiments and for exploring future avenues. The central questions of the proposal are related to the late time Rayleigh-Taylor (RTI) instability growth suppression using magnetic fields and the existence of a lower bound in the mix development. In seeking to address these questions, we will provide the first comprehensive studies using accurate numerical simulations of magneto-hydrodynamic (MHD)-Hall RTI with realistic plasma transport properties. We expect to be able to address questions related to mix properties and the possibility of controlling mix in Inertial Confinement Fusion as well as many questions relevant to a multitude of astrophysical configurations.

Technical Outcomes

We performed fully resolved simulations under a variety of configurations and late time Inertial Confinement Fusion (ICF) conditions to understand the role of the combined buoyancy, magnetic, and Hall effects on the Rayleigh-Taylor instability growth, turbulence, and mixing. The results show several surprising new physics and the importance of including plasma transport, as opposed to relying on numerical errors to model subgrid terms, and better resolved meshes in future calculations of ICF problems.

Publications

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Superconducting Nuclear Recoil Sensor for Directional Dark Matter Detection

Markus Hehlen
20150437ER

Project Description

We will model, fabricate, characterize, and assess a new solid-state sensor concept for the directional detection of dark matter. The work will provide the data needed to formulate a roadmap for the future development of a large-scale solid-state detector. The overall technical goal of the project is to demonstrate the novel concept of a layered glass/superconducting sensor for directional dark matter detection. We will (1) comprehensively model the nuclear recoil properties in the detector materials, (2) fabricate a single layered detector structure, (3) assess the sensitivity and directionality of the device using ion beams, (4) fabricate a multilayer prototype to assess scalability, and (5) measure the detector background performance. Results of this work will build underlying science and technology in areas of interest to nuclear nonproliferation, treaty verification, and global security where directional detectors can play a critical role.

Technical Outcomes

We have developed a novel concept of a directional dark-matter detector. Our model calculations indicate that the detector can have an excellent front-to-back signal ratio, potentially enabling the detection of the sidereal dark-matter flux variation on Earth. We have successfully demonstrated the fabrication and excellent performance of the superconducting niobium sensor. We expect to observe the transient response of the detector on a set of advanced samples to be characterized in a follow-on effort.

Publications

Junghans, A., N. Weisse-Bernstein, K. Baldwin, R. Lafler, N. Phan, D. Loomba, and M. P. Hehlen. Directional dark matter detection using superconducting nuclear recoil sensors. Presented at *APS March Meeting*. (Baltimore, MD, 14-18 Mar. 2016).

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Neutrinos and Fundamental Symmetries in Nuclei

Stefano Gandolfi
20150476ER

Project Description

We will employ Quantum Monte Carlo methods to evaluate weak matrix elements in light nuclei. Realistic interactions and currents have been used to describe many processes in light nuclei spectra, reaction rates, and electron scattering. At the completion of this project we will have a vastly improved capability to predict weak interaction rates for nuclei, both at the low energy and momentum scales relevant for beta decays, the moderate momentum transfer relevant for neutrinoless double beta decay matrix elements, and an accurate two-nucleon model for quasielastic neutrino scattering.

Technical Outcomes

We performed a fully quantitative prediction of electro-weak processes in light nuclei, including electron and neutrino scattering, and beta decay rates. Our predictions are in excellent agreement with available experimental data.

Publications

Lovato, A., S. Gandolfi, J. Carlson, S. C. Pieper, and R. Schiavilla. Electromagnetic and neutral-weak response functions of ^4He and ^{12}C . 2015. *Phys. Rev. C*. **91**: 062501. <http://link.aps.org/doi/10.1103/PhysRevC.91.062501>.

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Zhao, P. W., and S. Gandolfi. Radii of neutron drops probed via the neutron skin thickness of nuclei. 2016. *Phys. Rev. C*. **94**: 041302. <http://link.aps.org/doi/10.1103/PhysRevC.94.041302>.

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Klos, P., J. E. Lynn, I. Tews, S. Gandolfi, A. Gezerlis, H. W. Hammer, M. Hoferichter, and A. Schwenk. Quantum Monte Carlo calculations of two neutrons in finite volume.

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Lonardonì, D., J. Carlson, S. Gandolfi, J. E. Lynn, K. E. Schmidt, A. Schwenk, and X. Wang. Properties of nuclei up to $A=16$ using local chiral interactions. Submitted to *PHYSICAL REVIEW LETTERS*.

E. Lynn, J., I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, and A. Schwenk. Quantum Monte Carlo calculations of light nuclei with local chiral two- and three-nucleon interactions. To appear in *PHYSICAL REVIEW C*.

Next-Generation Double Beta Decay Experiment

Steven Elliott
20150088DR

Project Description

In this project, we will perform critical R&D to reduce the experimental and theoretical risks associated with next-generation experiments to search for double beta decay. Our expected results include assessments of new cryostat designs for germanium detectors, use of robotics in assessing detectors, new data acquisition techniques, understanding the depth requirement for such experiments, and key theoretical issues in nuclear and particles physics required to fully understand a measurement of double beta decay.

Technical Outcomes

We performed a number of studies that will improve the sensitivity of a future double beta decay experiment. This included theory of the underlying physics of the process, along with measurements to reduce background that might hide the signal. We built and tested apparatus for detector studies and Rn emanation measurements. We benchmarked simulations of the performance of underground laboratory performance against data to provide better predictive capability for future efforts.

Publications

Elliott, S. R., and H. Ejiri. Solar neutrino interactions with the double beta decay nuclei of ^{82}Se , ^{100}Mo and ^{150}Nd . 2017. *Phys. Rev. C*. **95**: 055501.

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J. A. Detviler, Dunagan, Efremenko, Ejiri, S. R. Elliott, Galindo-Uribarri, Gilliss, G. K. Giovanetti, Goett, M. P. Green, J. T. Gruszko, I. S. Guinn, V. E. Guiseppe, Henning, E. W. Hoppe, Howard, M. A. Howe, B. R. Jasinski, K. J. Keeter, M. F. Kidd, S. I. Konovalov, R. T. Kouzes, B. D. LaFerriere, Leon, A. M. Lopez, MacMullin, R. D. Martin, Massarczyk, S. J. Meijer, Mertens, J. L. Orrell, O'Shaughnessy, N. R. Overman, A. W. P. Poon, D. C. Radford, Rager, Rielage, R. G. H. Robertson, Romero-Romero, M. C. Ronquest, Schmitt, Shanks, Shirchenko, Snyder, A. M. Suriano, Tedeschi, J. E. Trimble, R. L. Varner, Vasilyev, Vetter, Vorren, B. R. White, J. F. Wilkerson, Wiseman, Xu, Yakushev, C. -. Yu, Yumatov, and Zhitnikov. Muon flux measurements at the davis campus of the sanford underground research facility with the MAJORANA DEMONSTRATOR veto system. 2017. *ASTROPARTICLE PHYSICS*. **93**: 70-75.

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KLYNAC Stability Study

Bruce Carlsten
20170669ER

Project Description

The goal of the project was to demonstrate a new architecture for generating a low energy (less than 6 million electron volts) electron beam. Conventional architectures require separate radio frequency (RF) sources and accelerator structures with complex RF connections and components, plus they require fine temperature control so that the RF source and accelerator structure operate at the same RF frequency. Our approach was to combine the RF source and the accelerator structure into a single structure (called a Klynac), which eliminates essentially all of that complexity. As a result, the klynac is a fraction of the weight and size of a conventional low-energy electron accelerator and can be fabricated for a fraction of the cost. The impact of this new device is broad. It can lead to a lightweight and portable accelerator for field operation such as for detection of special nuclear materials. For medical applications, the reduced size and weight of a klynac may significantly reduce the complexity and size of the cost-dominating gantries required for moving the radiation source about the patient. Finally, it can lead to a less expensive source of low energy electrons needed for science experiments, such as for studies of plasma-beam interactions.

Technical Outcomes

We successfully added $\sim 10\mu\text{H}$ of series inductance to the CLiA high-voltage modulator to shorten rise time. The CLiA modulator was not reliable at 50kV and failed at high-voltage despite several iterations of replacing electronics. As a result, we were unable to measure the decay of the klynac's parasitic RF modes. We believe the CLiA unreliability at high-voltage was due to years of accumulated stress operating at lower voltages, degrading the components and impacting reliability.

LCLS Harmonic Seeding Experiments to Improve Temporal Coherence of X-ray Free-Electron Lasers

Dinh Nguyen
20170621ER

Project Description

A novel method will be developed to improve the coherence of modern X-ray free-electron lasers (XFEL) and extend the XFEL photon energy into the hard X-rays that can be used to probe materials of interest to DOE/NNSA. The first method is based on seeding a two-stage XFEL with the harmonic radiation generated in the first stage after appropriately filtering out the fundamental radiation with an X-ray attenuator prior to seeding the second stage. We expect to see the proof of spectral narrowing with the new harmonic seeding technique in the collaborative experiments with SLAC using the Linac Coherent Light Source XFEL at SLAC. The second technique is based on manipulating the electron bunch and X-ray pulse to produce opposite correlations in energy-time and allowing them to interact in a new undulator called Transverse Gradient Undulator to produce a narrower spectrum in the XFEL output. The new seeding technique has the potential of delivering extremely bright XFEL laser beams with much improved temporal coherence, i.e., narrower spectral bandwidth. Using computer simulations, we show that we could generate an XFEL output spectrum that is narrower than the usual 0.1% relative bandwidth of a typical XFEL operating in the self-amplified spontaneous emission mode.

Technical Outcomes

We developed a new harmonic seeding technique to improve the temporal coherence (narrow-bandwidth) of X-ray free-electron lasers (XFEL) and extend the photon energy range beyond the hard X-ray region. Our method is based on a two-stage design where the coherent harmonic radiation generated in the first stage seeds the XFEL interaction in the second stage. The harmonic seeding technique can deliver coherent X-rays beams with improved spectral brightness compared to the currently used self-seeding technique.

Emma, C., Y. Feng, D. C. Nguyen, A. Ratti, and C. Pellegrini. Compact double-bunch x-ray free electron lasers for fresh bunch self-seeding and harmonic lasing. 2017. *Physical Review Accelerators and Beams*. **20** (3): 030701. <http://https://journals.aps.org/prab/pdf/10.1103/PhysRevAccelBeams.20.030701>.

Publications

Quantum Entanglement at Modern Colliders

Christopher Lee
20160644PRD1

Project Description

This project proposes to develop a robust theory of low-energy radiation between colliding protons that causes quantum entanglement, such that they cannot be treated as independent objects. We will remove from theory predictions the assumption that strongly interacting particles in high-energy collisions are free from effects of quantum entanglement. This will enable us to fully grasp strongly interacting particles as a many-body system quantum mechanically interacting in real time. Protons and nuclei form the ammunition for the collisions at Fermilab and others. Our work will bring under control the effects of entanglement on the theoretical prediction collisions outcomes and make them reliable probes for properties of nucleons, quark-gluon plasma, and signals for new physics. This addresses one of the top-level priorities called out by the Nuclear Science Advisory Committee.

Neill, D. The asymptotic form of non-global logarithms, black disc saturation, and gluonic deserts. To appear in *Journal of High-Energy Physics*. <http://arxiv.org/abs/1610.02031>.

Technical Outcomes

We made new discoveries about the dependence of proton-proton collision cross sections on correlated gluon emissions in separated regions. First we found a new way to organize the perturbative series in these emissions that converges uniformly, allowing more accurate predictions. Second, we uncovered a new relation between this series and nuclear parton distributions for large densities of soft partons, opening a new avenue to study factorization violating effects due to this soft structure of nucleons.

Publications

Neill, D., I. Scimemi, and W. J. Waalewijn. Jet axes and universal transverse-momentum-dependent fragmentation. Submitted to *Journal of High-Energy Physics*. <http://arxiv.org/abs/1612.04817>.

Larkoski, A. J., I. Moulton, and D. Neill. The analytic structure of non-global logarithms: convergence of the dressed gluon expansion. 2016. *Journal of High-Energy Physics*. **11**: 89. <http://arxiv.org/abs/1609.04011>.

Photocathodes in Extremes: Understanding and Mitigating High Gradient Effects on Semiconductor Cathodes in X-FELs

Nathan Moody
20140616ER

Project Description

This project quantifies the upper damage threshold, in terms of electric field, of semiconductor electron sources (cathodes) so that expensive x-ray free electron laser designs can be based on validated cathode test data, rather than assumptions. This research will answer fundamental questions concerning the behavior of electron beam sources (namely, upper limit of electric field) when subjected to the conditions associated with an electron beam based x-ray free electron laser (X-FEL). The results will include both fundamental research validating the basic approach to designing electron beam sources, and/or demonstrating the enabling technology required to successfully utilize those cathodes in a specific X-FEL design. Key technical challenges and solutions, such as cathode seal geometry and high electric field surface treatment, will emerge and the data will allow future X-FEL designs to be based on validated test results.

Technical Outcomes

The Cathodes in Extremes LDRD designed, fabricated and tested a high-electric-field gradient test cell (HGTC), intended to allow validation of novel photocathode materials and cathode-to-RF structure joints. Operated at the Argonne Wakefield Accelerator, the HGTC generated electric fields of up to 60 MV/m. The HGTC also demonstrated operation of a variable on-axis power coupler, a clamp-on temperature stabilization system and below-room-temperature operation.

Publications

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Electron Transport in Warm and Hot Dense Matter

Charles Starrett
20150656ECR

Project Description

The ultimate result of this work will be a completely new computational framework for calculating electrical conductivity in warm and hot dense plasmas. The method will compare favorably to the existing gold standard methods at low temperature, and provide the gold standard at higher temperatures, where none currently exists. The method will lead to a new understanding of electron transport in dense plasmas and the resulting calculations will be of high relevance to the modeling of inertial confinement fusion experiments (eg. at the National Ignition Facility).

Technical Outcomes

Two new computer codes were developed. The first calculates electrical conductivities in warm and hot dense matter based on an average atom formalism. Results from the code agree well with experiments and other sophisticated and much more computational expensive methods. The second code calculates the electronic structure of warm and hot dense matter using the KKR-GF method and has led to an enhanced Equation of State capability at the Laboratory.

Publications

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Transport Properties of Magnetized High-Energy Density Plasmas

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20150520ER

Project Description

We will develop a quantitative understanding of transport processes in magnetized high-energy density plasmas. Models of transport properties will be developed and validated using molecular dynamics simulations and practical expressions will be formulated. A critical component of realizing our energy and security missions relies on understanding high energy density plasmas (HEDP). Exciting recent research has demonstrated that strong magnetic fields provide substantial benefits that may accelerate progress toward milestones in these areas. Combining numerical simulations and analytical modeling, our efforts will enable a first-principles exploration of the transport properties of magnetized HEDP. Tangible products will be a numerical code and theory capable of describing these plasmas, and practical formulas that can be implemented into integrated simulation codes used to model inertial confinement fusion (ICF) systems.

Technical Outcomes

A critical component of realizing the Laboratory's energy and security missions relies on understanding high energy density plasmas (HEDP). Our efforts enable a first-principles exploration of the transport properties of magnetized high-energy density plasmas, especially in connection to current Inertial Confinement Fusion research. A simulation capability was developed to study how magnetic fields affect the transport properties of magnetized HEDP. A practical model was developed to accurately predict these transport properties.

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Probing New Sources of Time-Reversal Violation with Neutron Electric Dipole Moment

Takeyasu Ito
20140015DR

Project Description

This joint experimental and theoretical effort aims to probe new sources of time reversal violation with the electric dipole moment (EDM), which measures the separation of positive and negative charges within a system. Our study will be executed using the Los Alamos Ultracold Neutron (UCN) source. We will develop a new neutron EDM (nEDM) experiment with a sensitivity goal of 3×10^{-27} e-cm, a 10-fold improvement over the current limit. More specifically, we will upgrade the existing UCN source, which is expected to result in a 10-fold performance increase. The resulting UCN source improvement will benefit fundamental neutron physics experiments, actinide sciences, and detection technology.

Technical Outcomes

We have successfully upgraded the ultracold neutron source at Los Alamos National Laboratory, and demonstrated that it can provide a sufficient ultracold neutron density for a new neutron electric dipole moment experiment with a sensitivity goal of 3×10^{-27} e-cm. We have successfully performed a demonstration Ramsey resonance measurement. We have pioneered first-principles calculations of the neutron EDM induced by new physics and we have studied the impact of EDMs on Higgs boson properties.

Publications

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Neutron Star Mergers Revisited

Wesley Even
20150712PRD2

Project Description

We will implement a novel computational approach to simulate matter ejection and macronovae from neutron star mergers. The resulting simulations will take advantage of numerical algorithms being developed at Los Alamos to scale ten to one hundred times the resolution that current models are typically conducted. The models will also include microphysics (i.e. opacities) in which Los Alamos experts are currently leading their fields. These results will be critical for locating sources and interpreting the results of the first gravitational wave signals from advanced gravitational wave detectors, such as the Laser Interferometer Gravitational-wave Observatory (LIGO). This research could have profound impact on the detection of neutron star mergers. It will also impact nuclear physics because neutron star mergers have been recently shown to be the main site for the r-process nucleosynthesis.

Technical Outcomes

This ambitious project endeavored to accurately simulate dynamical ejecta from neutron star mergers and predict a new, previously undetected optical / IR transient: a macronova / kilonova. The project resulted in fruitful collaboration between atomic physicists, radiative transport and nucleosynthesis experts. The end product provided state-of-the-art models of macronovae, which have been successfully applied to recent ground-breaking observations, placing Los Alamos researchers among field leaders.

Publications

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Research Enabling a Next Generation Neutron Lifetime Measurement

Steven Clayton
20140568DR

Project Description

This project will develop and apply two major innovations to the study of neutron decay with ultracold neutrons. We will store very low energy neutrons in a magnetic bottle and observe the decay of these neutrons. Measuring the rate of the decay will tell us about how the matter forming our universe was formed, and the fundamental forces governing the physical world. This work will advance the Laboratory's ability to understand neutrons and make measurements with and about them, which is a core capability of the nuclear weapons and nuclear nonproliferation programs.

Technical Outcomes

This project resulted in a world's most precise single measurement of the neutron lifetime. In contrast to previous precision measurements of the neutron lifetime, systematic corrections are much smaller than statistical uncertainty. The method employed a novel trap for ultracold neutrons that eliminated material interactions during neutron storage. A new detector technology for ultracold neutrons was developed as part of this project and enabled high statistical efficiency and direct study of subtle systematic effects.

Publications

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Wang, M. A. Hoffbauer, C. L. Morris, N. B. Callahan, E. R. Adamek, J. D. Bacon, Blatnik, A. E. Brandt, L. J. Broussard, S. M. Clayton, Cude-Woods, Currie, E. B. Dees, Ding, Gao, F. E. Gray, K. P. Hickerson, A. T. Holley, T. M. Ito, C. Y. Liu, Makela, J. C. Ramsey, R. W. Pattie Jr., D. J. Salvat, Saunders, D. W. Schmidt, R. K. Schulze, S. J. Seestrom, E. I. Sharapov, Sprow, Tang, Wei, Wexler, T. L. Womack, A. R. Young, and B. A. Zeck. A multilayer surface detector for ultracold neutrons. 2015. *NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT*. **798**: 30-35.

Revolver: A Radical Inertial Confinement Fusion Ignition Design

Mark Schmitt
20170612ER

Project Description

We propose an alternate approach to ignition on the NIF that is characteristically different from existing concepts. Our innovative concept could be a game changer for the entire inertial confinement fusion (ICF) community, where the advancement toward ignition has been stalled by unresolved and unknown physics issues. Achieving ignition on NIF would be huge scientific accomplishment for Los Alamos, the ICF community and the nation. Ignition would also provide an unparalleled platform for future Stockpile Stewardship efforts at the national laboratories.

Technical Outcomes

Performance models for the innovative Revolver multi-shell ignition targets show that analytic hard-sphere illumination is an excellent predictor of implosion symmetry for symmetric laser geometries and are consistent with current National Ignition Facility (NIF) laser capabilities (were symmetric drive available). Analysis indicates that Revolver's shells should not break up from hydrodynamic instability growth and that inner shell mix with deuterium-tritium (DT) fuel appears to be small. These are important steps toward achieving ignition on NIF.

Publications

- Schmitt, M. J., K. Molvig, P. McKenty, and N. S. Krasheninnikova. Optimizing ICF fuel compression for NIF using a directly-drive multiple-shell liquid-fuel concept. 2017. *To be submitted to Physics of Plasmas.*
- Molvig, K., M. J. Schmitt, T. A. Gianakon, P. McKenty, E. M. Campbell, and R. Betti. Persistent stagnation and high efficiency burn in a Revolver capsule. 2017. *To be submitted to Physics of Plasmas.*

Multi-Scale Kinetics of Self-Regulating Nuclear Reactors

Venkateswara Dasari
20150058DR

Project Description

We propose to investigate the use of tuneable micro-scale materials to achieve self-regulation in small compact reactors with numerous national security implications. This project aims to develop a disruptive solution based on the premise that dispersed fuel composites can be tuned at the micro-scale such that emergent neutron behavior can be designed to self-regulate a reactor with minimal control systems or human intervention. Operationally, the Defense Science Board identified small compact reactors to be "game-changers" whose demand cannot be underestimated for space exploration, underwater vehicles, assured arctic awareness, and satellites that can operate on the dark side of the globe. This research will demonstrate feasibility and readiness of such a technology for near-term use.

Technical Outcomes

This project demonstrated the feasibility of self-regulating nuclear reactors for space and remote applications. Nuclear fuel with specific functionality was designed, analyzed and fabricated. A promising high temperature hydride moderator was fabricated and tested. Nuclear physics experiments required to demonstrate the performance were designed. A multi-scale and multi-physics analysis tools set were developed. New self-regulating reactor designs were developed to demonstrate value of the underlying technologies. Significant interest exists to commercialize these technologies.

Publications

- Hurley, D., E. P. Luther, and I. O. Usov. Spatially Resolved Thermal Transport Measurements in PyC Coated Fuel Particles. Presented at *Transaction of American Nuclear Society*.(New Orleans, LA, August 2016).
- Usov, I., and D. V. Rao. Pyrolytic Carbon Coatings on Oxide and Carbide Microspheres. 2016. In *Proceedings of TMS 2016: the Materials and Fuels for Advanced and Current Nuclear*

Reactors.(Orlando, FL, November 2016). Vol. Supplemental Proceedings, p. 40. Nashville, TN: Springer.

- Cummins, D. R., E. Luther, A. Telles, and P. Pappin. Low Temperature Sintering of Silicon Carbide for New Self Regulating Reactor Design. Presented at *Rio Grande Fuels Conference*.(Los Alamos/ Albuquerque, September 2015).
- D. V. Rao, E. Luther, Fabrication and Characterization of Graphite Composite with Controlled Thermal and Mechanical Properties. Presented at *TMS 2016*.(Orlando, November 2016).

Optimization of Compton Source Performance through Electron Beam Shaping

Nikolai Yampolsky
20150690ECR

Project Description

This project aims to investigate in detail the possibility of increasing the quality of light sources that utilize relativistic electron beams. The key challenge is finding the optimal distribution of electrons that results in the brightest light source. We expect to demonstrate that inverse Compton scattering (ICS) brightness can be increased through appropriate conditioning of the electron beam phase space. We expect to eliminate the largest contribution to the brightness degradation, i.e. either due to the angular divergence or the energy spread of the electron beam. At the moment, it is an open question whether both effects can be suppressed simultaneously. We conservatively anticipate that only one of them can be compensated and the final source brightness will be defined by the smallest rather than the largest effect. Recently, high-flux gamma rays have been proposed as approaches for detecting special nuclear materials and to address international nuclear proliferation concerns. A compact ICS source is an attractive option for generating these photons.

Technical Outcomes

The single-electron Wigner distribution function of the light emitted in the ICS was derived for the first time. This result has been used to find the Wigner distribution function of radiation emitted by an ensemble of electrons with an arbitrary distribution in the phase space. The results show that the peak brightness of the ICS source can be increased on the order of 4 orders of magnitude for typical electron beams.

Publications

Malyzhenkov, , and Yampolsky. Optimization of Compton Source Performance through Electron Beam Shaping. 2017. *ADVANCED ACCELERATOR CONCEPTS*. **1812**.

Malyzhenkov , A. V., and N. Yampolsky. Optimization of Compton Source Performance through Electron Beam Shaping. 2016. In *North American Particle Accelerator Conference* .(Chicago, 10/9/16-10/14/16). p. 474. Chicago, IL: AIP.



Science of Signatures

Discovering Biosignatures in Manganese Deposits on Mars

Nina Lanza
20160606ECR

Project Description

On Earth, high concentrations of manganese are associated with life and environments supportive of life. Our goal is to identify key signatures pointing to a biological origin for manganese-rich materials so they may be identified on Mars by rovers. The objective of this project is to determine what chemical and mineralogical signatures can uniquely identify manganese-rich materials as biological in origin using Mars rover payload instruments. 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

Oyen, D. A., and N. L. Lanza. Interactive machine learning for discovering patterns in spectral data and images. 2017. In *3rd Planetary Data Workshop*.(Flagstaff, AZ, 12-15 June 2017). p. no. 7054. Houston, TX: Lunar and Planetary Institute.

Oyen, D. A., and N. L. Lanza. Automatically identifying rock coatings in laboratory LIBS data using machine learning algorithms. 2017. In *48th Lunar and Planetary Science Conference*.(The Woodlands, TX, 20-24 March 2017). p. no. 1479. Houston, TX: Lunar and Planetary Institute.

Lanza, N. L., S. M. Clegg, A. Cousin, O. Forni, M. F. Kirk, S. N. Lamm, A. M. Ollila, V. Payre, and R. C. Wiens. Identifying potential chemical biosignatures in manganese minerals with laser-induced breakdown spectroscopy. 2017. In *48th Lunar and Planetary Science Conference*.(The Woodlands, TX, 20-24 March 2017). p. no. 2913. Houston, TX: Lunar and Planetary Institute. <http://https://www.hou.usra.edu/meetings/lpsc2017/pdf/2913.pdf>.

Oyen, D., and N. Lanza. Interactive discovery of chemical structure in ChemCam targets using Gaussian graphical models. 2016. In *Workshops of the International Joint Conference on Artificial Intelligence (IJCAI)*.(New York, NY, 10 July 2016). p. N/A. N/A: N/A. <http://users.sussex.ac.uk/~nq28/beyondlabeler/OyeLan16.pdf>.

Additive Manufacturing of Composite Lithium Containing Neutron Scintillators

Markus Hehlen
20160678PRD4

Project Description

We will develop and demonstrate the additive manufacturing of a composite neutron scintillator for the first time. The resulting material is expected to enable a new class of neutron detectors needed for a wide range of national-security applications. Key metrics of success include the scintillator performance and the projected manufacturing cost. We anticipate that the resulting composite scintillator will out-perform any other neutron detector in terms of gamma-ray rejection and sensitivity per volume. We also anticipate that the projected scintillator manufacturing cost will make this novel detection approach economically competitive with existing neutron detectors such as He-3 tubes.

Accumulator for Low-Energy Laser-Cooled Particles

Kevin Mertes
20160584ER

Project Description

The technical base of accumulators and injectors for high-energy particles can be molded into exotic experiments or medical tools. Analogous elements, we will show, can also be made for ultracold matter, for use in a wide and newfound range of research. Accumulators are special tools of high-energy physics (HEP) that catch and overlap batches of particles into dense packets. Accumulator principles, however, are not exclusive to HEP and may be formed for the decidedly low-energy particles of laser-cooled atoms and molecules, as indicated by our calculations. We propose to build an accumulator for cold atoms and demonstrate its capacity for gathering more cold particles than possible by conventional means and concentrating them to very high densities. With greater familiarity and adoption, accumulators could provide a foundation for applications of ultracold matter in navigation, precision measurement, remote sensing, and chemical detection.

Publications

Mertes, K. M., P. Walstrom, and M. D. DiRosa. Accumulator for Low-Energy Laser-Cooled Particles . Presented at *48th Annual Meeting of the American Physical Society Division of Atomic, Molecular and Optical Physics*.(Sacramento, CA, 5-9 June 2017).

Narrow Spectrum Gamma-Ray Production Through Inverse Compton Scattering with a Free-Electron Laser

Frank Krawczyk
20160459ER

Project Description

We will determine the fundamental limitations to very narrow gamma-ray production through inverse Compton scattering. This is needed for the future capability to detect special nuclear material through nuclear resonance fluorescence. The technical goals are to demonstrate a novel inverse Compton scattering/free-electron laser (FEL) hybrid approach to generating MeV gamma rays with spectral widths of 0.1% and less and to develop a validated predictive capability through detailed measurements at the Lawrence Livermore accelerator facility. We will be able to produce high flux gamma rays with an order of magnitude narrower spectral widths than ever before, allowing us to experimentally investigate subtleties and the interdependencies of the various physical phenomena leading to gamma ray spectral broadening.

Publications

Carlsten, B. E., F. L. Krawczyk, J. W. Lewellen, Q. R. Marksteiner, D. C. Nguyen, and N. A. Yampolsky. High repetition-rate inverse Compton scattering x-ray source driven by a free-electron laser. 2014. *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*. **47** (23).

Novel Antennas Based on Atomic Magnetometers

Malcolm Boshier
20160518ER

Project Description

We will use new atomic magnetometer technology to develop compact high-performance receiving antennas. These devices have applications relevant to the intelligence community. The overall technical goal is to show that newly developed atomic magnetometer technology can realize low-frequency receiving antennas with an unprecedented combination of high sensitivity and compact size. Unclassified applications of these devices include communication underground, through buildings, and under water; receiving signals from low frequency beacons; and remotely diagnosing machinery operating in an underground facility.

Publications

Savukov, I. M., and M. G. Boshier. A high-sensitivity tunable two-beam fiber-coupled high-density magnetometer with laser heating. 2016. *Sensors*. **16**: 1691. <http://www.mdpi.com/1424-8220/16/10/1691>.

Using Extinct Radionuclides for Radiochemical Diagnostics (U)

Hugh Selby
20160011DR

Project Description

The goals of the Extinct Radionuclide System (ERS), that is, the integrated measurement, simulation and analysis tools for debris diagnostics, are simple but offer significant positive impact to all missions that employ radiochemical debris data. The single most important goal is to develop the suite of diagnostically useful measurement signatures that have been lost to decay. Validation of the measurements against known examples is the corollary of the main goal and will prove the feasibility of ERS concept. Successful development of the ERS will mark a completely new capability to address a number of NNSA missions. In essence, anything that one would do with fresh debris can now be done with old debris. This has major implications for the NNSA's main mission, Stockpile Stewardship. This statement can be understood by considering that all data employed in modern Stewardship is decades old and reflects the precision and accuracy of that time. The ERS allows for much more data and much higher precision. Such improvements will provide the data backstop for more confident stewardship assessments. These same ERS tools can be applied to other missions in the National Security endeavor, including treaty monitoring and verification.

Publications

Buescher, K. L. (U) Device degeneracy and capture reactions. 2017. *Internal LANL report (LA-CP-17-00071)*.

Parsons, D. K. Some notes on neutron up-scattering and Doppler broadening of high-Z scattering resonances. 2017. *Internal LANL report (LA-CP-17-28809)*.

Hanson, S. K., A. D. Pollington, C. R. Waidmann, W. S. Kinman, A. M. Wende, J. L. Miller, J. A. Berger, W. J. Oldham, and H. D. Selby. Measurements of extinct fission products in nuclear bomb debris: Determination of the yield of the Trinity nuclear test 70 y later. 2016. In *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*. Vol. 113, 29 Edition, p. 8104.

Meininger, D., S. K. Hanson, and C. R. Waidmann. Measurements of extinct Ag-111 in trinitite. 2017. *Manuscript in preparation*.

Range-Resolved Measurement of Atmospheric Greenhouse Gases for Treaty Verification and Climate Science

Brent Newman
20160462ER

Project Description

We will demonstrate a novel scheme to measure atmospheric gas concentrations in the stratosphere between 15 and 30 km altitude. This measurement technique can be flown in a satellite and may support future greenhouse gas treaty verification. The technical goal of this project is to verify our hypothesis that we can use a W-Band approach to interrogate the stratosphere for volume-constrained spectroscopy of atmospheric gases. Using available hardware, we will separately verify the two key elements in this hypothesis: (1) the Rayleigh reflection of aerosols in the stratosphere between 15 and 30 km altitude at W-band is large enough so a practical spectroscopy instrument can be built, and (2) by measuring the differential absorption of a specific gas rotational resonance at slightly different altitudes, we can determine the gas concentration at that altitude. Both climate science (in particular modeling of greenhouse gases) and future greenhouse gas emission treaty verification will greatly benefit from this new technology.

Radio Frequency Scintillation Prediction Driven by Direct Measurement of Ionospheric Spatial Irregularities

Max Light
20160231ER

Project Description

Scintillation, or distortion and degradation of a radio signal as it passes through the ionospheric plasma, is a concern for space-based nuclear detection. This project will help determine the viability of a new scintillation prediction method. There is currently no global system to measure electron density at the spatio-temporal scales required for scintillation prediction. This project will provide a system architecture and proof-of-concept for such a system. Once implemented, measurements from the proposed system will aid in answering global scintillation questions and could be part of a global scintillation forecasting system. The ability to accurately predict scintillation effects with our model will advance the design of space-based sensors used to detect signals generated from a nuclear detonation.

Publications

Lay, E. H. Ionospheric acoustic and gravity wave activity above low-latitude thunderstorms. Submitted to *Geophysical Research Letters*.

Probing Critical Behavior in Hydraulic Injection Reservoirs and Active Seismic Regions

Paul Johnson
20160144ER

Project Description

Conspicuously, seismicity rates in the mid-west United States have dramatically increased over the last 10 years, corresponding to the rapid growth of unconventional oil and gas production and the associated fluid waste injection. A moderate or large magnitude earthquake located in or near a population center could be potentially catastrophic. If a probe existed for the critical stress state at locations in which earthquakes may occur, preventative action (such as termination of pumping) could be taken. We propose that dynamically triggered microearthquakes can be used as a probe of critical stress state (faults near failure) within injection reservoirs and active tectonic regions, and aim to develop the methodology to quantify the new probe. This work could dramatically advance earthquake hazard analysis for both natural and anthropogenic earthquakes.

Publications

Delorey, A. A., N. J. van der Elst, and P. A. Johnson. Tidal triggering of earthquakes suggests poroelastic behavior on the San Andreas Fault. 2017. *EARTH AND PLANETARY SCIENCE LETTERS*. **460**: 164-170.

Delorey, A. A., M. Maceira, E. M. Syracuse, D. Coblenz, R. Guyer, and P. A. Johnson. The State of Stress at Intermediate Scales. 2017. In *Seismological Society of America Annual Meeting*. (Denver, 18-20 April 2017). Vol. 88, p. 689. Albany, CA: Seismological Society of America.

Van der Elst, N., A. Delorey, D. Shelly, and P. Johnson. Fortnightly modulation of San Andreas tremor and low-frequency earthquakes. 2016. *P.N.A.S.* **113**: 8601-8605.

Deep Learning for Multispectral and Hyperspectral Target Detection in Remote Sensing Data

Monica Cook
20170537ECR

Project Description

Target identification from remote sensing imagery is already recognized as a potential solution to a number of high-profile national security problems and DOE/NNSA missions. The goal of this research is to improve upon current results in order to extend this utility to other applications of great importance. We expect by the end of this research to understand how deep learning can be utilized to improve current performance in target detection from remote sensing imagery. The product will be a processing chain that can analyze large volumes of spectral remote sensing imagery quickly and efficiently using deep learning to achieve improved target identification results. Using new techniques to resolve current challenges will improve the accuracy of a solution that will continue to be demanded to solve important problems.

Integrated Biosurveillance

Benjamin McMahon
20150090DR

Project Description

We will apply three types of diagnostics to characterize emergence of disease and antibiotic resistance in an immunocompromized population living in the high-disease-burden area of western Kenya. This project will lay the foundations to achieve our long-term technical goals of situational awareness for global pathogen circulation and emergence, thereby addressing national security missions in the area of biological threat reduction. We will apply three types of diagnostics to characterize emergence of disease and antibiotic resistance in an immune-compromised population living in the high-disease-burden area of western Kenya. Our approach involves biomarker discovery, assay development, and assay deployment of three complementary infectious disease assays on a human population. Overall information integration and process optimization will result from both statistical analysis and development and application of realistic epidemiological models. If successful, this work could enable characterization of emerging diseases in the high-disease-burden region where they emerge.

Publications

- Brown, M., L. Moore, B. McMahon, D. Powell, M. LaBute, J. Hyman, A. Rivas, M. Jankowski, J. Berendzen, J. Loeppky, C. Manore, and J. Fair. Constructing rigorous and broad biosurveillance networks for detecting emerging zoonotic outbreaks. 2015. *PLoS ONE*. e0124037. <http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0124037>.
- Xie, G., J. Z. Kubicek-Sutherland, P. K. Dighe, L. L. Jacobs, H. Daligault, K. Davenport, Q. Cheng, P. Kempaiah, V. Otieno, E. Raballah, S. Anyona, C. Ouma, D. J. Perkins, H. Mukundan, B. H. McMahon, and N. A. Doggett. Comparative genomic and phenotypic characterization of invasive non-typhoidal Salmonella isolates from Siaya, Kenya. 2017. *Submitted to PLoS Pathogens*.
- Doggett, N. A., Mukundan, E. J. Lefkowitz, T. R. Slezak, P. S. Chain, Morse, Anderson, D. R. Hodge, and Pillai. CULTURE-INDEPENDENT DIAGNOSTICS FOR HEALTH SECURITY. 2016. *HEALTH SECURITY*. **14** (3): 122-142.
- McMahon, B., P. Fenimore, S. Del Valle, N. Hengartner, R. Ribeiro, and J. Hyman. Modeling the impact of spatial heterogeneity, behavior change, and mitigations on the current Ebola epidemic. 2015. *LAUR 14-27813*.
- McMahon, B. H., Hengartner, Mukundan, Voter, Jakhar, J. M. Ong'echa, Kempaiah, Karim, and D. J. Perkins. DISEASE-SPECIFIC CYTOKINE PROFILES IN PEDIATRIC PATIENTS WITH MALARIAL, HIV, AND SYSTEMIC BACTERIAL INFECTIONS. 2017. *AMERICAN JOURNAL OF TROPICAL MEDICINE AND HYGIENE*. **95** (5): 405-405.
- Stromberg, L. R., H. M. Mendez, S. W. Graves, N. W. Hengartner, and H. Mukundan. Presentation matters: impact of conformation of amphiphilic LPS on innate immune signaling. To appear in *PLoS ONE*.
- Noormohamed, , L. R. Stromberg, A. S. Anderson, Karim, Dighe, Kempaiah, J. M. Ong'echa, D. J. Perkins, Doggett, McMahon, and Mukundan. Detection of Lipopolysaccharides in serum using a waveguide-based optical biosensor. 2017. *OPTICAL DIAGNOSTICS AND SENSING XVII: TOWARD POINT-OF-CARE DIAGNOSTICS*. **10072**.
- Stromberg, L. R., N. W. Hengartner, K. L. Swingle, R. A. Moxley, S. W. Graves, G. A. Montano, and Mukundan. Membrane Insertion for the Detection of Lipopolysaccharides: Exploring the Dynamics of Amphiphile-in-Lipid Assays. 2016. *PLOS ONE*. **11** (5).
- Mendez, H. M., L. R. Stromberg, Swingle, S. W. Graves, Montano, and Mukundan. Serogroup-specific interactions of lipopolysaccharides with supported lipid bilayer assemblies. 2017. *BIOPHYSICS, BIOLOGY AND BIOPHOTONICS II: THE CROSSROADS*. **10075**.
- Davenport, G. C., J. B. Hittner, Otieno, Karim, Mukundan, P. W. Fenimore, N. W. Hengartner, B. H. McMahon, Kempaiah, J. M. Ong'echa, and D. J. Perkins. Reduced Parasite Burden in Children with Falciparum Malaria and Bacteremia Coinfections: Role of Mediators of Inflammation. 2016. *MEDIATORS OF INFLAMMATION*.
- Noormohamed, , Stromberg, Karim, Dighe, Wren, Gans, Perkins, McMahon, Doggett, and Mukundan. DETECTION OF SALMONELLA BACTEREMIA IN RURAL KENYA USING FIELDABLE DIAGNOSTICS. 2017. *AMERICAN JOURNAL OF TROPICAL MEDICINE AND HYGIENE*. **95** (5): 528-528.

Vu, D. M., A. Noormohamed, H. M. Mendez, L. R. Stromberg, D. J. Perkins, and H. Mukundan. Measuring host lipoprotein associated lipopolysaccharides in serum: implications for direct diagnosis of Gram-negative sepsis. Submitted to *PLoS ONE*.

Deshpande, , McMahon, A. R. Daughton, E. L. Abeyta, Hodge, Anderson, and Pillai. SURVEILLANCE FOR EMERGING DISEASES WITH MULTIPLEXED POINT-OF-CARE DIAGNOSTICS. 2016. *HEALTH SECURITY*. **14** (3): 111-121.

Kubicek-Sutherland, J. Z., A. C. Hengartner, and H. Mukundan. Membrane insertion for direct detection of lipoteichoic acid. 2017. *Transactions of the Materials Research Society of Japan*. **42** (4): 101-105.

Kubicek-Sutherland, J. Z., D. M. Vu, H. M. Mendez, S. Jakhar, and H. Mukundan. Detection of lipid and amphiphilic biomarkers for disease diagnostics. 2017. *Biosensors*. **7** (3): 1-25. <http://www.mdpi.com/2079-6374/7/3/25/htm>.

Developing a Compact Portable Muon Tracker for Non-Destructive Evaluation

Elena Guardincerri
20160629ECR

Project Description

We propose to design and build a modular muon tracker for radiographing thick structures and imaging denser objects inside those structures. The tracker will be capable of recording data and tracking muons with a good angular resolution. We will characterize our detectors by measuring the accuracy of the muon tracks reconstructed from the data, and we will leak test the drift tubes periodically and evaluate their long-term performances.

Publications

Gaal, R. Unveiling the past with nuclear physics . 2017. *APS News*. **26** (4): 1. <http://https://www.aps.org/publications/apsnews/201704/upload/APS-News-April-2017.pdf>.

Del Mauro, D. Tracking muons to reduce nuclear threats and help preserve architectural treasures. 2016. *Physics Flash*. **March**: 1. http://https://www.lanl.gov/org/padste/adepts/physics/_assets/docs/physics-flash-march-2016.pdf.

Guardincerri, E. Muons in the cathedral. 2017. *Santa Fe New Mexican*. 10.

A Novel Ultrasound Tomography Technique for High-Resolution Imaging

Lianjie Huang
20170203ER

Project Description

This research will advance the Laboratory's world-leading acoustic-wave and elastic-wave capabilities, which are crucial for addressing various challenges in energy and environmental security, nuclear security (monitoring weapon components), and public health. With this project, we endeavor to develop the first transrectal ultrasound tomography technique to accurately distinguish malignant from benign prostate tissues, and aggressive from indolent or nonaggressive prostate cancers. Results from this project could fill a technology gap identified by the U.S. Preventative Services Task Force for new imaging techniques; in fact, there is great opportunity for multi-mission impact due to the technology's safe (non-ionizing radiation), cost-effective, and portable imaging modality.

Publications

- Huang, L., K. Gao, and Y. Huang. Transrectal ultrasound-waveform tomography using plane-wave reflection data for prostate cancer imaging. To appear in *2018 SPIE Medical Imaging*. (Houston, TX, 10-15 Feb. 2018).
- Shin, J., Y. Lou, J. T. Yen, and L. Huang. Spatial Prediction Filtering for Increased Penetration Depth in Synthetic Aperture Ultrasound. 2017. In *2017 IEEE International Ultrasonics Symposium*. (Washington, D.C., 6-9 September, 2017). p. . New York: IEEE.

Agile Spectral Reconnaissance from CubeSats

Steven Love
20170055DR

Project Description

Remote chemical analysis by spectral remote sensing is an extremely powerful tool for both national security and earth science problems. Deploying this capability in space, however, has traditionally demanded national-level investment and many-year development efforts. This project seeks to enable a paradigm shift to rapidly deployable, inexpensive constellations of CubeSats. These fully functional miniaturized satellites are small enough to hold in your hand, game changingly inexpensive to launch, and carry ultra-compact spectral imagers that ultimately could provide comparable sensing capability with far greater agility and far lower cost. This project jumpstarts this vision by rapidly building and launching a high-performance CubeSat-based hyperspectral imager, operating in the ultraviolet/visible spectral region, to perform targeted mapping of key signature gases. This first demonstration focuses on earth science problems: volcanic gas monitoring for eruption prediction and greenhouse gas tracking via the easily detected proxy gas nitrogen dioxide. However, with anticipated improvements in CubeSat pointing accuracy, CubeSat-based instruments capable of detecting gases and materials of relevance to proliferation detection and other national security problems should be possible. This project lays the groundwork for future low-cost and versatile multi-CubeSat monitoring constellations.

Publications

Theiler, J., B. Foy, C. Safi, and S. P. Love. On-board CubeSat processing for hyperspectral gas detection. Presented at *SPIE Defense and Security, Algorithms and Technologies for Multispectral, Hyperspectral, and Ultraspectral Imagery XXIV*. (Orlando, 15-19 April, 2018).

Coherent Radio Frequency Collection Through Computation for CubeSat Constellations

Zachary Baker
20170583ER

Project Description

The goal of this project is to change how we think about and build arrays of satellites. Traditional radio collection vehicles required large dish receivers; this means large, expensive satellites. Our approach breaks the large satellite into many small apertures and then computationally recombines the observations of the small satellites. The key promise of "agile space" is that a medium number of low-cost vehicles orbited can provide similar functionality but with multiple eggs in multiple baskets. These clusters of small satellites are very hard to target, "cheap" to replace, and provide higher coverage over Earth for longer periods of time with increased survivability

Publications

Baker, Z., N. Dallmann, and B. Junor. Aperture Synthesis from Free-flying Collectors without Accurate Metrology. To appear in *IEEE Aerospace Conference*. (Big Sky, MT, 3 Mar 2018).

Fieldable Chemical Threat Mapping by Multi-Modal Low Magnetic Field Nuclear Magnetic Resonance Signatures

Robert Williams
20170048DR

Project Description

Over the past 90 years we have successfully made chemical agents more lethal, harder to destroy, and easier to obtain and use. Today, thousands of chemicals have the potential to be used as weapons of mass destruction. By extending Los Alamos National Laboratory's extensive expertise in high field Nuclear Magnetic Resonance (NMR) signature detection and ultra-low magnetic field relaxometry and Magnetic Resonance Imaging, our team has taken an innovative approach using multi-modal NMR signatures to unequivocally characterize and identify Chemical Warfare Agents (CWAs), their precursors and degradation compounds, as well as related Chemical Threat Agents (CTAs) and emerging threats. A transformative, innovative, and portable technology detects vulnerabilities and threats through unique, multiple Nuclear Magnetic Resonance (NMR) signatures that conclusively identify CWAs and other emerging threats allowing them to be mitigated. Our new measurement capabilities and strategies will map human activities in manufacturing and/or the use of toxic chemicals, pesticides, pharmaceuticals, and explosives as well as assist in responding to the accidental release of such chemicals or the intentional release by terrorists. With the ever-changing national and global security environment, these advances will mitigate vulnerabilities and keep pace with the rapidly evolving security environment that is affected by hazardous chemical misuse.

Quantum-Dot-Based Infrared Photodetectors with Picosecond Temporal Resolution Operating at Room Temperature

Istvan Robel
20170435ER

Project Description

The principal goal of this project is to develop inexpensive, high-efficiency, and high-time-resolution infrared photodetectors based on semiconductor quantum dots, a class of nanomaterials with size-tunable optical and electronic properties. Such technologies could find applications for surveillance, remote sensing, and spectral imaging.

Laser Radiochronometry

Alonso Castro
20170199ER

Project Description

The goal of this project is to demonstrate the development of a new method for dating nuclear materials, i.e., the determination of the date when a nuclear material, such as uranium or plutonium, was first manufactured and purified. This new method will improve upon existing radiological dating methods such as mass spectrometry because it is fast, inexpensive, and will be able to date materials without signal interferences from isotopes of similar masses, such as ^{241}Pu and ^{241}Am .

Elpasolite Planetary Ice and Composition Spectrometer (EPICS): A Low-Resource Combined Gamma-Ray and Neutron Spectrometer for Planetary Science

Laura Stonehill
20170438ER

Project Description

The Elpasolite Planetary Ice and Composition Spectrometer (EPICS) will provide a transformational advance in the orbital investigation of the composition of planetary bodies, including asteroids, moons, Mars, and the inner planets. The elpasolite scintillators and other new technologies in EPICS enable for the first time combined neutron and gamma-ray spectroscopy with a single detector, yielding a substantial reduction in instrument size, mass, power, and complexity for future planetary science missions. Planetary science provides high-profile positive press to the Laboratory, raising our scientific visibility and attracting new talent. EPICS will also revitalize synergy between planetary science and national security in space. Neutron and gamma-ray planetary science instruments have significant design synergy with instrumentation for the US Nuclear Detonation Detection System (USNDS) program and other national security missions; staying engaged in scientific instrument development is critical for retaining talent, remaining abreast of new technologies, and improving future USNDS instrument designs.

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Inspecting America's Aging Infrastructure with Muon Radiography

J Durham
20170402ER

Project Description

As our country's infrastructure continues to age and deteriorate, America is increasingly subject to economic losses from process downtime as well as loss of competitiveness in the global industrial market. Los Alamos National Laboratory has developed a new, unique method to non-destructively evaluate industrial components, using only naturally occurring background radiation from space called "cosmic ray muons." Using these particles, we can produce tomographic images of pipes, valves, concrete, and other object that can be subject to aging and failure. Unlike x-rays, this method does not rely on artificial sources of radiation that may give workers or the public unnecessary exposure. Muons are also highly penetrating, enabling inspections of (for example) pipes that are covered by insulation while they are in use. For a typical x-ray or ultrasound inspection, insulation must be removed prior to inspection, and the process using that pipe must be stopped. Since muons can image deterioration through insulation, there is no downtime associated with this technique. This new inspection technique can be applied to power plants, petrochemical refineries, and multiple other industrial sites. Reduced process downtime and increased confidence in our country's infrastructure will result in economic benefit to the United States.

Fluctuating Domains in Antiferromagnets for Sensing and Switching Applications

Vivien Zapf
20170288ER

Project Description

Technology is moving beyond simple ferromagnets, where all the individual electron spins align with each other. New computing, sensing, communication and energy technologies are increasingly using antiferromagnets and more complex magnetic structures, where the different spins point in different directions and break various symmetries. As these useful magnets become more complex, it becomes challenging to study them. In particular, we need to understand defects, domains, and fluctuations in antiferromagnets and other complex magnets. It is well established that domains control the functionality of ferromagnets. Domains are likely very common in antiferromagnets as well, however they have historically been difficult to study. Here we explore how the new generation of magnetic field and X-ray technologies at DOE and NNSA facilities in conjunction with world-class theoretical efforts can be applied to understanding domains and fluctuations in antiferromagnets. This work extends our fundamental understanding of technologies related to communication, energy, data storage and manipulation and sensing.

Publications

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High Energy Lightning: Understanding Relations Between Energetic Particles and Lightning Discharges in Thunderclouds

Xuan-Min Shao
20170179ER

Project Description

This project directly addresses DOE/NNSA's 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.

Publications

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Walking the Road from Impacts to Seismic Sources for Celestial Bodies

Carene Larmat
20170109ER

Project Description

The goal of this project is to facilitate future seismic missions to a multitude of planets and moons. Decades of seismic exploration on Earth has provided high-resolution images of its buried features, and we know that important clues to natural resources of other planets will reside in their interior. However, data return from extraterrestrial seismic missions is highly dependent on how efficient are impacts to generate seismic waves. The level of uncertainty of current models translates in high risk explaining the low number of seismic missions launched by NASA so far. This view is changing as the Discovery program gears towards planets beyond Mars. This research aims to provide a new generation of numerical Bolide impact models for rocky planets. These models will leverage on unique modeling capabilities developed at Los Alamos to capture the high-strain high-energy physics involved in modeling of Underground Nuclear Explosions (UNEs). Of note, the new material models developed will extend our nuclear monitoring ability to unconventional geologic environments (i.e. other than US and Russian test areas), which will help address new threats emerging for the DOE monitoring mission.

Publications

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Point of Care Enabling Technologies(PoCET): Magnetically Coupled Valves & Pumps

Pulak Nath
20170026ER

Project Description

This project is enabling the development of the "liquid logic" technology, which is essentially the reduction of common laboratory processes into handheld platforms that are fully automated and deployable for point of care applications. Proposed work supports the "forward deployment" theme of the Los Alamos Science of Signature pillar. From medical diagnostics to nuclear forensics, the capabilities developed with this project will support a wide range of applications. Microfluidics have experienced remarkable growth with thousands of patents/publications in the last 15 years. Nevertheless, in most cases we get "chip-in-a-lab" as opposed to "lab-on-a-chip," due to large peripherals such as pumps, valves, tubes, electrical/optical components, and sensors. Our focus is to develop miniaturized magnetically coupled microfluidic valves, pumps, and their novel driver mechanism. These platforms will enable truly integrated microfluidic platforms that can carry out complex operations in a pocket size platform, which otherwise would require significant laboratory space with current technologies.

Publications

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Life on the Edge: Microbes in Rock Varnish

Chris Yeager
20170414ER

Project Description

This project supports DOE's Energy Security mission by conducting basic research on exoelectrogenic processes (the extracellular electron transfer pathways that allow certain microorganisms to transfer energy between intracellular chemical energy stores and extracellular solids) under harsh conditions. Additionally, this research benefits NNSA's mission in nonproliferation because elemental signatures in rock varnish can be used to characterize past atmospheric depositional events. By integrating Los Alamos capabilities and expertise in geochemistry, space science, and microbiology we aim to: 1) identify and interpret the microbial species and processes involved in the habitation and/or formation of rock varnish; 2) identify organic biosignatures that, in concert with trace element and mineralogy, can be used to conclusively distinguish the biogenic and abiogenic origins of terrestrial Mn-rich surfaces; 3) determine the role of light-dependent Fe/Mn redox chemistry in sustaining life in rock varnish. Each of these goals in and of themselves has important implications for our understanding of how life on Earth has evolved to capture and harness energy from the physical environment, and will aid in our search for similar processes on Mars. Knowledge gained from this research will benefit further technological advances in DOE-relevant fields ranging from bioenergy to solar energy to bioremediation.

10 Gigahertz Bandwidth Synthetic Aperture Radar (SAR) Technology Development for Satellite Deployment

Bruce Carlsten
20160013DR

Project Description

We will develop a radio frequency (RF) amplifier with order-of-magnitude higher power and bandwidth than possible with conventional technology at extremely high frequency to enable ultra high resolution imaging for urgent national security missions. RF amplifier technology has a performance limitation at high frequency because sizes shrink, including the size of the electron beam needed for RF amplification. It has been long recognized in the RF amplifier technical community that a sheet electron beam will be needed to bypass this limitation, but previous research has shown that sheet beams with conventional RF structures lead to over-moding. This project proposes to demonstrate a high-frequency RF amplifier using novel high-dielectric constant ceramics. These ceramics will allow the development of RF amplifier designs that eliminate mode competition yet have unprecedented wide bandwidths.

Publications

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Strontium Bose-Einstein Condensate Atom Interferometer with Matter Wave Circuits

Changhyun Ryu
20170218ER

Project Description

Inertial navigation is essential in many national security missions. Although GPS-based navigation can be used in ideal situations, when GPS service is denied or unavailable, an independent, accurate, inertial sensor is needed. Traditional technologies have reached their limit in sensitivity and a new approach has been sought. Inertial sensing with an atom interferometer is a promising new direction to improve sensitivity in sensing of rotation and acceleration toward the goal of long distance navigation without GPS input. We will develop a novel inertial sensor with atoms trapped in a waveguide made of laser beams. Since atoms are trapped inside waveguides, the interrogation time can be very long and this increases sensitivity accordingly. The successful completion of this project will demonstrate the highest sensitivity in sensing of rotation and acceleration with waveguide atom interferometer. This will make it possible to develop a portable compact inertial sensor for many national security missions. This research is relevant to DOE/NNSA missions of national security science in developing novel sensing technologies for national security missions.

Three-Dimensional Nuclear Quadrupole Resonance Imaging

Petr Volegov
20170141ER

Project Description

This work will result in a new method to non-invasively detect and image illicit substances (namely explosives and narcotics) at a chemically specific level. While many other imaging techniques exist, none are able to positively identify specific chemical compounds, making our approach a unique tool for substance detection. With immediate national security applications in airport security, IED detection and removal, and drug trafficking, there is a large application space for our technology. Our principal goal is to demonstrate the first 3D image with our two proposed techniques and determine the ultimate physical limits of our approach. Specific to NNSA, our research has the potential to look inside the bulk high explosives of our nuclear warheads to address questions about aging and quality control of the manufacturing process to ensure the safety and suitability of our stockpile for years to come.

Time-of-Flight Ion Mass Spectrometer Subsystem for Space and Planetary Missions

Herbert Funsten
20160440ER

Project Description

This project proposes to advance ultrathin foil technology with graphene and reflectron technology with precision-resistive coatings. We will develop and demonstrate two enabling technologies that allow Los Alamos to retain leadership in space mass spectrometry and energetic neutral atom (ENA) imaging. The combination of these two technologies in a mass spectrometer subsystem will enable future leadership on several missions to study Earth, planets, and the Sun's interaction with the interstellar medium. The technologies are also applicable to ground-based and laboratory high mass resolution time-of-flight mass spectrometers. This work has application to mission challenges in the area of space situational awareness.

Technical Outcomes

This project developed and demonstrated the process for fabricating high quality graphene films and the optimized transfer process to an open grid for use in space energetic neutral atom imagers and mass spectrometers. The project also developed a method for deposition of graded resistance coatings on the interior of a plastic cylinder drift region of a time-of-flight mass spectrometer, enabling unprecedented mass resolution.

Signature Development in Los Alamos National Laboratory's Earth and Space Sciences

Reinhard Friedel
20150647DR

Project Description

This project expands the scientific understanding of fundamental physical processes that are critical to maintenance of habitat earth homeostasis with the long-term objective of achieving sufficiently detailed knowledge to identify the tipping points that can push habitat earth out of its homeostatic equilibrium. This scientific goal is achieved by promoting and coordinating basic research based on the science of signatures to gain understanding of the structure, and evolution of the earth, the solar system and the Universe in which habitat earth resides, ultimately relevant to understanding future changes as they might perturb habitat Earth homeostasis. The science of signatures and the means to detect and interpret these signatures is directly applicable to the detection needs for nonproliferation and counter proliferation community, space weather and space events, remote sensing and detection of chemical, biological, nuclear, radiologic, or explosive threats, climate impact and treaty verification, and cosmology/astrophysics. Signature discovery and alternate signatures provide the new methods to detect and understand these areas of national need.

Technical Outcomes

This project executed 57 separate tasks leading to advances in strategic areas of Geoscience (Earth's State of Stress, slip prediction machine learning, kinematic permeability inversion from seismic signatures), Astrophysics (Planet formation, astrophysical jet formation in the lab, dark matter detection with HAWC), Climate (Environmental Effects through bird microbiome studies, insect outbreak induced forest mortality, imaging tree roots) and Space Physics (Electron accelerators in space, spacecraft charging solutions, real time radiation belt models).

Publications

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Chemical Signatures of Detonation Born From Extreme Conditions (U)

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20150050DR

Project Description

We will combine novel methodologies to understand how solid carbon forms and evolves during detonation with state-of-the-art analysis of detonation debris. Traditional nuclear forensic investigations provide little or no insight into the dynamics of high explosive detonation. Post-detonation and real-time signatures of explosive test programs and unique materials identifiers are needed, but can only come from a fundamental understanding of the physical processes that lead to their formation and evolution in time. Successful execution of this project will provide models critical to improved weapons simulation and results could prove useful in DOE/NNSA defense and nuclear nonproliferation programs.

Technical Outcomes

We established an interdisciplinary effort to understand how solid carbon forms and evolves during detonation, developed new models to describe its evolution, and linked in-situ measurements of signature formation with post-detonation characteristics. Recovery studies on well-controlled tests indicate that high explosive formulation, detonation atmosphere, and test design (pressures and temperatures reached during detonation) influence final recovered products as indicated by size, surface structure, fractal dimension, morphology, and elemental and isotopic composition of the detonation soot.

Publications

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Mapping Relativistic Electron Precipitation: Where and When?

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20150127ER

Project Description

We aim to map regions of electron loss in the Van Allen radiation belts using a novel technique that combines point measurements from a large number of satellites to remotely sense the location of the loss and properties of waves driving the loss. Electron precipitation has been shown to affect telecommunications and atmospheric chemistry, and plays a critical role in determining radiation belt dynamics; it is therefore a key process to understand for space weather modeling. Our primary objective is to demonstrate that point measurements from a constellation of satellites can be combined to remote sense, and hence map, regions of loss. Our secondary objective is to use these data to infer key properties of a type of electromagnetic wave responsible for driving some of the losses. This will produce new physical understanding, enable scientific studies not previously possible and provide critical inputs for radiation belt models.

Technical Outcomes

Electron fluxes from the Global Positioning System (GPS) constellation have been improved and cross-calibrated against the Van Allen Probes mission and phase space densities have been calculated. Novel techniques for analyzing data across a diverse constellation have been developed, allowing monitoring of an electron drift shell. A data-optimized magnetic field model has been developed. Statistical analysis and simulations have been employed to study radiation belt dynamics and the occurrence of waves that determine losses.

Publications

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Ultra-sensitive Parallel Micro-imaging with Atomic Magnetometer

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20150300ER

Project Description

We will construct and characterize a sensitive magnetic-imaging device capable of microscopic resolution. Various applications will be developed for biosecurity, industry, energy science, brain science, and cancer research. This project will address needed improvements in both resolution and sensitivity for the application of magnetometry in biological and neuroscience applications. We propose to do this via a novel approach: combining an ultra-sensitive atomic magnetometer (AM) with flux concentrators (FCs). After the FC-AM devices have been tested and characterized, we will work on developing novel applications. We will demonstrate detection of magnetic nano-particles functionalized for specific molecules. Nano-particle applications are relevant to Los Alamos missions in security, energy research, and nonproliferation.

Technical Outcomes

We developed an ultra-sensitive magnetic microscope based on an atomic magnetometer and ferromagnetic flux guides. Demonstrated high sensitivity and resolution will enable many novel applications, such as single neuron detection, magnetic nano-particle detection for cancer diagnostics, and many others. We also designed a multi-channel magnetometer and performed simulation for an array of flux guides proving the possibility of multi-channel parallel imaging. The capability has spurred several follow-on projects.

Publications

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Exploiting Cross-sensitivity by Bayesian Decoding of Mixed Potential Sensor Arrays

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20150236ER

Project Description

This project will build an electrochemical sensor array and algorithms that will enable the detection of specific chemical signatures in a complex gas mixture. The array will be demonstrated in vehicle exhaust monitoring and explosives detection. We propose to use a special class of ceramic solid-state electrochemical sensors that are intrinsically inexpensive, durable, and stable. Nobody has ever attempted to create a sensor array using these devices before. Their robustness opens the possibility of detecting a great number of gas chemistries under conditions that would quickly destroy other types of electronic noses. The proposed research has the ability to create a unique capability at Los Alamos National Laboratory by supporting the development of inexpensive and portable systems for use both by civilian first responders and as dedicated screening systems at airports, federal buildings, cargo containers, etc.

Technical Outcomes

Laboratory mixed-potential electrochemical sensor (MPES) device arrays were coupled with advanced Bayesian inference treatment of the physical model of relevant sensor-analyte interactions. We demonstrated that our approach could be used to uniquely discriminate the composition of ternary gas sensors with three discreet MPES sensors with an average error of less than 2%. We also observed that the MPES exhibited excellent stability over a year of operation at elevated temperatures in the presence of test gases.

Publications

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Low-cost High-resolution Sensing and Health Monitoring of Urban Infrastructure

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20150708PRD2

Project Description

This project focuses on developing a low-cost, rapidly deployable system for measuring the dynamic response of structures. It is expected that this work will be applicable to monitoring the condition of urban/energy infrastructure. This project aims to develop the signal processing tools and techniques needed to enable the use of imagers to perform structural inspections. If successful, the work has potential to remove the energy, bandwidths and installation problems associated with conventional structural health monitoring measurement networks because in a number of cases a few imagers may be able to collect data that is roughly analogous to the data collected by a dense sensor network consisting of accelerometers and strain gauges. This would be a great step toward the widespread adoption of structural health monitoring.

Technical Outcomes

This project developed an algorithm to blindly and automatically extract high-resolution mode shapes of a structure from video. This algorithm/technique can detect the presence of very small (3%) loss-of-stiffness in a structure and estimate cable tension. This capability - an extremely sensitive technique available for remotely detecting structural loss-of-stiffness using low-cost, commercially available video cameras - improves the nation's ability to monitor the condition of urban/energy infrastructure, monitor manufacturing, and respond to disasters.

Publications

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Trojan Horse Drug Development Approach: Targeting Gene Dosage Control to Induce Bacterial Suicide

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20150664ECR

Project Description

In this project we seek to discover a novel class of antimicrobial therapies that can restrict the evolution of drug resistant pathogenic bacteria. To achieve this goal, we propose to elucidate a poorly understood mechanism for regulation of protein turnover in the bacterial cell. Messenger ribonucleic acids (RNA) translate the genetic information stored on deoxyribonucleic acid (DNA) molecules into amino acid sequence in the proteins. Discovery of therapeutics that can restrict the emergence of drug resistant pathogenic bacteria would have a high impact on drug development and national security.

Technical Outcomes

Multi-drug resistant bacteria present a threat to public health. Our work paved the way to the discovery of a novel class of antibiotics that can restrict the evolution of drug resistant bacteria through inhibition of the selective cleavage of ribonucleic macromolecules, RNA, by RNaseE. We found 25 FDA approved therapeutics and food supplements to act on the interface of protein-RNA interaction. These compounds will serve as scaffolds for the rational design of novel antimicrobial agents.

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Development of Radiation Detector Simulation Framework and Safeguards Instrumentation

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20150705PRD2

Project Description

This work will advance technology for international safeguards through characterization and testing of a safeguards instrument, as well as development of general simulation tools that will be used with that instrument. The resulting coherent stand-alone tool for detector simulation will be designed to be coupled to the Los Alamos National Laboratory radiation transport simulation software MCNP. The tool will provide a framework for implementation of detector simulations for a wide variety of radiation detector types. The tool will be validated using data from measurements taken with the safeguards instrument.

Technical Outcomes

This work contributed to nuclear safeguards instrumentation development and simulation capabilities. The iSFRC instrument, intended to measure fuel being discharged from nuclear reactors, has been fully assembled with new data acquisition hardware, and tested for gamma and neutron response. This project also resulted in the development of DRiFT (a Detector Response Function Toolkit). DRiFT provides a flexible framework for nuclear instrumentation simulations, and has contributed to several ongoing projects at the Los Alamos National Laboratory.

Publications

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Remote Raman and Laser-Induced Breakdown Spectroscopy (LIBS) Analysis of Geologic Samples Under Venus Surface Conditions

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20170568ER

Project Description

The focus of this research project was to develop and demonstrate the remote Raman and Laser-Induced Breakdown Spectroscopy (LIBS) methods required to investigate chemical and mineralogical compositions under simulated Venus surface conditions. The new remote Raman and LIBS (RLS) spectrometer suite was used to probe geochemical and mineralogical standards at a 2 m standoff distance. Most importantly, the propagation of a 1064 nm laser through a potentially turbulent atmosphere was investigated experimentally and theoretically. The Venus surface is a 92 atm. supercritical fluid at 463°C. While a lander will warm up over the ~ 1 hour descent to the surface, there will still be small differences in the lander and Venus surface temperatures, especially at the window through which the RLS instrument will be directed. We found that a LIBS plasma can be routinely generated even when the temperature difference exceeds 60°C. Finally, we designed a compact RLS instrument for future Venus surface investigations. These results also demonstrate that RLS can be used on other samples under extreme conditions related to the Los Alamos mission.

Technical Outcomes

The project demonstrated that LIBS and Raman spectroscopy are capable of rapidly acquiring the chemical and mineralogical compositions under Venus surface conditions and are consistent with the preliminary theoretical LIBS calculations. The integrated computational fluid dynamics (CFD) and optical model clearly demonstrated that the LIBS laser will focus to the laser spot size required to generate a plasma. Finally, we designed a RLS instrument capable of fitting within the limited space of a Venus lander.

Ignis: A Cognitive Radio Frequency Sensing Low-Probability-of-Detection-and-Interception Modem

Joseph Palmer
20170538ER

Project Description

The armed forces of the United States of America face increasingly hostile radio frequency (RF) environments that are expected to threaten its ability to maintain open lines of communication during a time of armed conflict. The threats are principally from new and advanced forms of electronic warfare in which potential adversaries are making significant R&D investments. Los Alamos possesses advanced wireless communication systems with low-probability-of-detection-and-interception (LPDI) capabilities. Originally developed for its nanosatellite program, these digital radio modems have excess computational capacity for the implementation of sophisticated signal processing and machine learning algorithms. The Ignis project studied how to exploit these strengths in order to incorporate cognitive radio technologies into the Laboratory's LPDI modems, thus addressing US armed forces' need for robust battlefield communication systems. The project outcomes were: 1) A novel interference mitigation technology, 2) a mutually cognitive radio communications concept, and 3) preliminary design of a manpackable cognitive LPDI modem for small-unit military forces. Development of the Ignis concept continues. When complete, the technology will be made available to government organizations that are searching for new and innovative ways of protecting US wireless communication systems.

Technical Outcomes

The project resulted in design of the Ignis Manpackable low probability of detection and interception (LPDI) spread spectrum modem, including a new requirement for emissions power control. The modem is ready for further detailed design, responding to national needs. The project also developed the Spectropuncher interference mitigation filter. It uses an unconventional iterative filter synthesis algorithm, has low implementation cost, good scalability, and

equivalent/better performance than existing techniques. A provisional patent application has been initiated.

Hand-held Laser-Ultrasound Two-Dimensional Scanner

Eric Flynn
20150673ECR

Project Description

This project proposes to develop and demonstrate a hand-held laser ultrasound scanner for rapid, stand-off inspection. The device will be designed to be carried by a person and operated by a single hand. The scanner will provide raw steady-state response measurements with more fidelity and at faster speeds than present, commercial, off-the-shelf laser Doppler vibrometry technology. It will seamlessly measure transitions between scanned components in an assembly and automatically map scan lines to physical space. Enabled technologies would include mobile robotic inspection platforms, "ultrasonic fingerprint" readers, tamper-indicating scanners, inspection of hard-to-reach components, inspection of component assemblies, emergency and quick-check inspections, and in-line manufacturing quality control.

Technical Outcomes

We developed a new compact ultrasound generator, all-fiber laser Doppler vibrometer (LDV) system, and hand-held pose-estimation and mapping system, culminating in a prototype. We expanded the application space to sandwich composites, additive manufacturing, material phase detection, and crack detection. It produced two non-provisional patents, two journal papers, six conference papers, and five invited talks. It led to a new project with Chevron, new collaborations with Lockheed Martin and NASA, and a one-year LDRD ER.

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Ultra-Sensitive Micro-Magnetic Imaging Endoscope

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20150701PRD1

Project Description

This project aims to develop cutting-edge technology for micro-magnetic imaging with applications from bio-security, to cancer detection, and single-neuron level functional imaging. We expect to demonstrate magnetic sensing with micro-mechanical resonators. In addition, sensing based on atomic spins will be explored. Imaging, either with scanning method or with multi-channel readout, will be tested. After initial demonstrations, we will focus on applications. We will demonstrate the detection of magnetic micro or nano-particles. Then we will try to demonstrate the measurement of neuronal activity. Tagged magnetic nanoparticle detection with the proposed technology will be of interest to biosecurity applications (pathogen detection) and medical diagnostics (cancer detection).

Savukov, I., J. Zhu, K. Henderson, A. Castro, and V. Lebedev. Trace Uranium Plutonium Mixture Characterization Using 3D Printed Optical Micro-resonators. 2016. *LDRD ER proposal*.

Technical Outcomes

The major outcomes are the construction of a whispering-gallery mode (WGM) testing platform, demonstration of a high magnetic-field sensitivity of robust polymer-encapsulated WGM sensor, demonstration of a liquid-state WGM magnetometer and studies of liquid-state WGMs, and demonstration of high-quality 3D printed WGMs. We introduced a new capability of WGMs to the laboratory. This capability enables applications in the area of high-sensitivity sensing, including mission-relevant applications, such as characterization of U and Pu mixtures.

Publications

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