Los Alamos National Laboratory

Laboratory Directed Research and Development
FY21 Annual Progress Report

Los Alamos
NATIONAL LABORATORY

N N S A
National Nuclear Security Administration

TRIAD
National Security, LLC

LDRD
LABORATORY DIRECTED
RESEARCH & DEVELOPMENT

Structure of this Report

The Laboratory Directed Research and Development (LDRD) Annual Report for fiscal year 2021 (FY21) is organized as follows:

Overview: A description of the LDRD program at Los Alamos National Laboratory (LANL), including the program's structure and objectives; a summary of the program's value; and highlights of outstanding program accomplishments.

Project Summaries: The project summaries are organized by Capability Pillar – Complex Natural and Engineered Systems, Information Science and Technology, Materials for the Future, Nuclear and Particle Futures, Science of Signatures, and Weapons Systems. Project summaries for continuing projects appear first, followed by project summaries and technical outcomes for projects that ended in FY21.

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

On the Cover

Cover image (Top left): LDRD researcher Victor Klimov has made great strides with Colloidal quantum dots. Learn more in this [article](#) in *Nature*. (Klimov, 20200213DR)

Cover image (Top center): RNA particles swarm an X chromosome from a mouse in a new visualization of X chromosome inactivation. [Read more](#). (Sanbonmatsu, 20210134ER)

Cover image (Top right): Machine learning models developed by several LDRD researchers are presented in this [cover article](#) in the *Journal of Physical Chemistry Letters*. (Barros, 20200209ER; Nebgen, 20210087DR)

Cover image (Middle left): For many years, Los Alamos scientists have been optimizing algae growth for biofuels and bioproduct development. This expertise is now key to developing the next generation of bioplastics. [Read more](#). (Marrone, 20190001DR)

Cover image (Middle center): LDRD researcher Victor Klimov has made great strides with Colloidal quantum dots. Learn more in this [article](#) in *the Journal of the American Chemical Society*. (Klimov, 20200213DR)

Cover image (Middle right): Pictured here is an open furnace containing molten salt: a clear, watery liquid at 800 degrees Celsius. LDRD researcher Marisa Monreal has established multiple new actinide-molten salt capabilities. [Read more](#). (Monreal, 20210113DR)

Cover image (Bottom left): LDRD researcher Victor Klimov aims to realize an electrically pumped laser with a solution processable gain medium. Pictured here is an artistic impression of red, green and blue lasers based on solution-processed colloidal quantum dots applied to a thin, flexible substrate. [Read more](#). (Klimov, 20210176ER)

Cover image (Bottom center): Early Career LDRD researcher Michael Peterson is using thundercloud illumination by lightning to understand optical signal propagation in nature. [Read more](#). (Peterson, 20200529ECR)

Cover image (Bottom right): This image shows two halves of an experimental aerogel sphere. New materials, specifically aerogels like the polyimide used in this three-inch prototype, may be key to air buoyant vacuum vessels. [Read more](#). (Beaux, 20190119ER)

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Leadership Perspectives

Bill Priedhorsky, LDRD Program Director

Every day, LDRD delivers technical vitality, mission agility and workforce development. The portfolio ranges from the applications side, where for example our Design for Manufacture project opens the door for new efficiencies in production, to the most fundamental research on the nature of life and matter. That fundamental work may decades hence deliver benefit to national security. In the interim, it builds the Laboratory's reputation and draws to these mesas the world's best and brightest. One of my mentors, the late Col. Terry Hawkins, spoke many times of deterrence by reputation – when the open accomplishments of a Lab like Los Alamos prove to the world that we can do amazing things, would-be adversaries will understand that the same capabilities stand ready for the nation's defense. In his words, if Los Alamos can detect neutrons on the Moon, our adversaries should know that Los Alamos can detect nuclear goings-on on the surface of this planet.

I am confident about the legacy that we have built. What we have done together in LDRD will reverberate for years to come. It has been my honor to lead the Laboratory Directed Research and Development program at Los Alamos since 2007. However, the time has come, as it always does, to hand the responsibility to someone else. While it is not easy to step away from LDRD, with its unique connection to the breadth of the Laboratory, it is time for me to do so.

After a rigorous search, the Deputy Director for Science, Technology, and Engineering has selected Laura Stonehill as the incoming Program Director. Laura has served as deputy LDRD Program Director for over 3 years; she arrived at the Laboratory as a Director's Postdoctoral Fellow (LDRD-supported, of course), in 2005, and contributed to fundamental (neutrino physics) and applied (national security instrumentation) R&D, before serving as program manager for space intelligence. Her experience in and out of LDRD will serve the program well.

While my direct involvement with LDRD is reaching its end, my retirement will not be a goodbye, but the next step in an engagement with the Laboratory that started in 1978. I will remain engaged as a retired Laboratory Fellow, doing what I can to help the Laboratory, its mission, and its incoming generation of talent.

LDRD has been the best job and greatest challenge of my career. I have been humbled by the commitment to excellence that I have encountered every day of those years. Working side by side with outstanding colleagues, we have taken LDRD to new levels of excellence, relevance, and rigor, building the future of this great Laboratory one project at a time.

> "LDRD is central to Los Alamos science, technology, and engineering strategy as articulated in our Laboratory Agenda and through our Capability Pillars, and I cannot imagine being successful without it. Our LDRD objectives of advancing technical vitality, mission agility, and workforce development align with and derive from this strategy. Because of LDRD's importance we must also ensure that we execute our LDRD program with the highest standards of transparency, objectivity, and inclusion, and an unwavering commitment to robust peer review."
> – **John Sarrao**, Deputy Director for Science, Technology, and Engineering

Laura Stonehill, incoming LDRD Program Director

I wish to thank and commend Bill Priedhorsky for his many years of dedication to LDRD. The program is strong and effective due to the rigorous processes, deliberate structure, and unwavering dedication to excellence developed under his leadership.

I am honored to have the opportunity to serve as the new LDRD Program Director. Managing this inspiring program is a challenge that I am truly excited to take on. I will bring a passion for science, technology, and engineering in support of LANL missions to my leadership of LDRD. I am fully dedicated to ensuring that LDRD strengthens the technical vitality, mission agility, and workforce development of the Laboratory by funding innovative research and development in forefront areas relevant to the entire breadth of LANL capabilities and missions. Under my leadership, LDRD will maintain our commitment to technical excellence and will increase efforts towards transparency of our processes, engagement with the breadth of the Laboratory, and diversity, equity, and inclusion.

In FY21, the LDRD program continued to grow with the Laboratory's increasing mission responsibilities. We were able to fund more of our flagship multidisciplinary Directed Research projects and our most forward-looking Exploratory Research (ER) projects than ever before. We built capabilities to solve key mission problems and address priorities in the Laboratory Agenda. At the same time, we piloted ER Seedling projects that provide the opportunity to address the highest-risk aspects of particularly innovative ideas, a recommendation from the FY20 ER Refresh.

LDRD has been exploring ways to simultaneously streamline and improve the rigor and objectivity of our peer review processes across the entire LDRD program, both in proposal review and project appraisals. An example is reducing the potential for bias through anonymous review of ER pre-proposals. These process adjustments will be refined going forward, in keeping with LDRD's spirit of continuous improvement.

LDRD Directives, Objectives, and Strategic Challenges

Laboratory Directed Research and Development (LDRD) at Los Alamos helps Los Alamos National Laboratory solve national security challenges through excellence in mission-focused science, technology, and engineering. The Laboratory and Site-Directed Research and Development programs are among the most impactful sources of research and development for our Nation. At Los Alamos, Lawrence Livermore, and Sandia National Laboratories, the Laboratory Directed Research and Development (LDRD) programs are important sources of internal investment in science and technology for the future. The Nevada National Security Site (NNSS) conducts applied science and technology research and development through the congressionally authorized Site-Directed Research and Development (SDRD) program. The LDRD and SDRD programs follow strategic guidance derived from the missions of the U.S. Department of Energy, the National Nuclear Security Administration (NNSA), and the Laboratory.

To execute that strategy, the Los Alamos LDRD program creates a free market for ideas, drawing upon the creativity of the Laboratory's best and brightest researchers. The combination of strategic guidance and grassroots competition provides a continual stream of capabilities that position the Laboratory to enable agile responses to national security challenges.

Funded with less than 6 percent of the Laboratory's operating budget, the LDRD program makes it possible for our scientists and engineers to pursue cutting-edge research and development in support of mission. This in turn helps the Laboratory, and the Nation, maintain its position of scientific and technological leadership.

LDRD objectives guide the program overall and align with DOE Order 413.2C Chg1. The LDRD program has three objectives: Technical Vitality, Mission Agility, and Workforce Development.

The Program's Objectives Align with DOE Objectives for LDRD

Technical Vitality	Mission Agility	Workforce Development
Advance the frontiers of science, technology, and engineering.	Enable agile responses to national security challenges.	Attract, develop, and retain tomorrow's technical workforce.

In 2019, DOE/NNSA prepared a [Strategic Framework for the Laboratory- and Site-Directed Research and Development program](#), which communicates NNSA's strategy for developing science and technology tools and capabilities to meet current and future national security challenges. The 2019 LDRD/SDRD Strategic Framework was drafted to convey the vision and objectives of the program and to demonstrate the firm commitment of NNSA leadership to the program.

The LDRD program responds to four national security challenges identified in the Strategic Framework (and derived from the 2018 Nuclear Posture Review).

The Program Responds to Four National Security Challenges

1. *Provide an agile, flexible, and effective nuclear deterrent.*
2. *Protect against all weapons of mass destruction threats.*
3. *Deter and defend against threats in multiple domains.*
4. *Strengthen our energy and environmental national security.*

This report will illustrate the Los Alamos LDRD program's success in responding to the National Security Challenges and meeting the LDRD objectives noted above.

LDRD Program Values

How we do our work is as important as what we do, in LDRD and elsewhere. The Laboratory assumes the responsibility for stewarding public resources when it oversees the LDRD program. When it succeeds, it delivers the nation full worth in all three objectives. Rigor in LDRD oversight reinforces the reputation of the Laboratory and the LDRD program. LDRD processes, though complicated in some details, are therefore driven by a small set of underlying values based on a commitment to excellence, transparency, and diversity/inclusion, all consistent with the Laboratory's [values](#).

LDRD Aligns with Laboratory Strategy

LDRD is essential for the technical vitality of the Laboratory and builds capabilities for future mission challenges. The Laboratory's Capability Pillars define strategic investment areas at Los Alamos for present and future missions. All LDRD investments are aligned with the Capability Pillars. See the Appendix for a project-by-project summary where projects are categorized by Capability Pillar.

Beginning with proposal calls released in FY21, LDRD aligns with all six Pillars. Note: Prior to FY21, LDRD aligned with "Focus Areas," rather than directly to the Capability Pillars. The Capability Pillars also form the strategic basis for the annual Strategic Investment Plan (SIP), which principally informs LDRD's flagship investment component–Directed Research.

The Capability Pillars Define Six Key Areas of ST&E in which the Laboratory Must Lead

CAPABILITY PILLARS	
MATERIALS FOR THE FUTURE	Defects and Interfaces Extreme Environments Emergent Phenomena
NUCLEAR AND PARTICLE FUTURES	Applied Nuclear Science & Engineering Nuclear & Particle Physics, Astrophysics & Cosmology Accelerator Science & Technology High Energy Density Physics & Fluid Dynamics
INTEGRATING INFORMATION, SCIENCE, AND TECHNOLOGY FOR PREDICTION	Computing Platforms Computational Methods Data Science
SCIENCE OF SIGNATURES	Nuclear Detonation Nuclear Processing, Movement, Weaponization Natural and Anthropogenic Phenomena
COMPLEX NATURAL AND ENGINEERED SYSTEMS	Human–Natural System Interactions: Nuclear Engineered Systems Human–Natural System Interactions: Non-Nuclear
WEAPONS SYSTEMS	Design Manufacturing Analysis
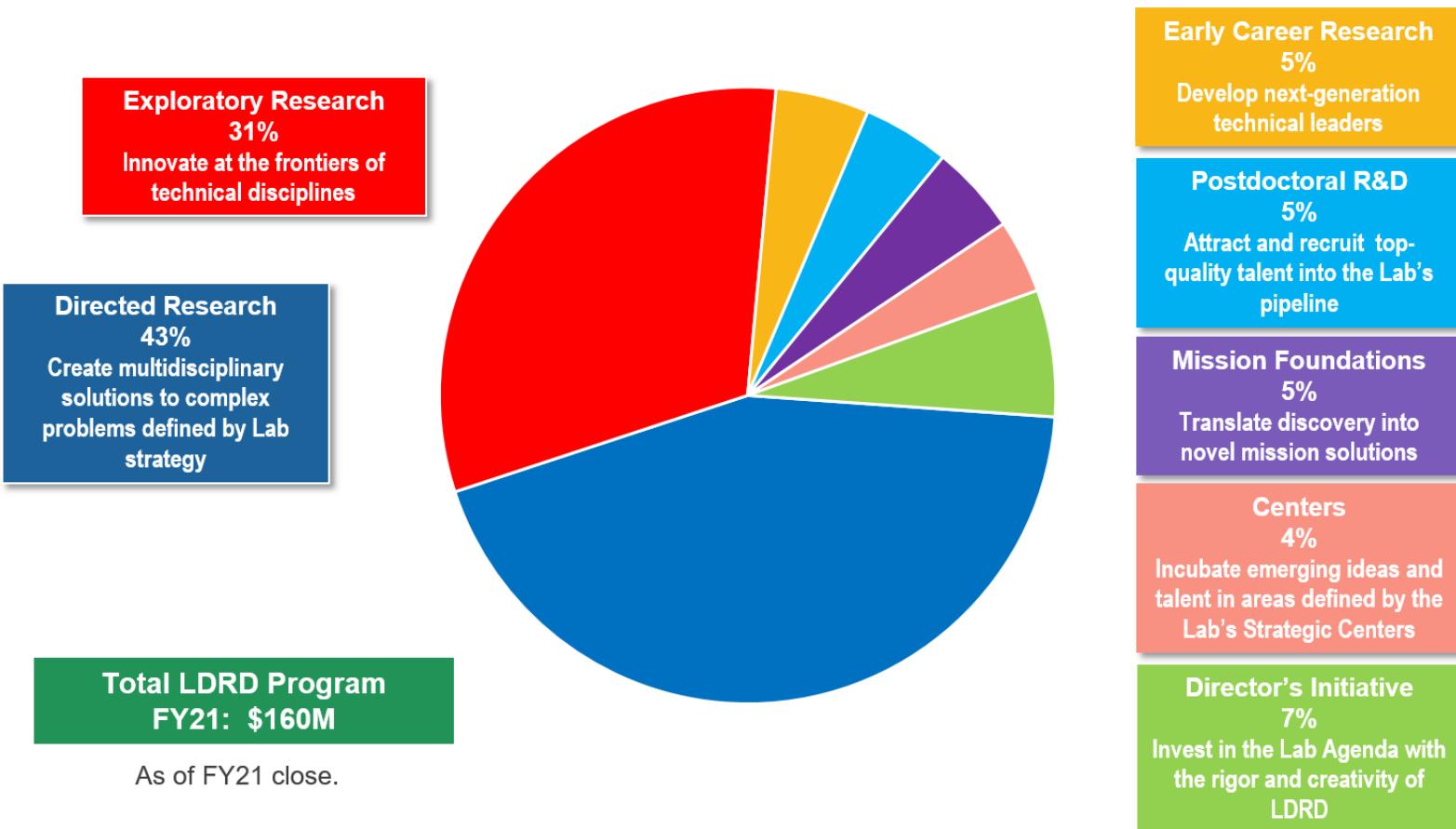
Program Structure
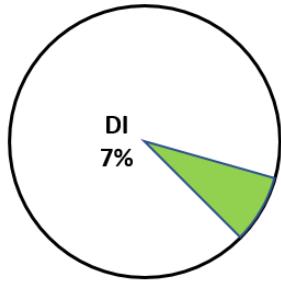
Overview

The Los Alamos LDRD program is organized into seven components with distinct institutional objectives: Directed Research (DR), create multidisciplinary solutions to complex problems defined by Lab strategy; Exploratory Research (ER), innovate at the frontiers of technical disciplines; Early Career Research (ECR), develop next-generation technical leaders; Postdoctoral Research and Development (PRD), attract and recruit top-quality talent into the Lab's pipeline; Mission Foundations Research (MFR), translate discovery into novel mission solutions; Director's Initiatives (DI), invest in the Lab Agenda with the rigor and creativity of LDRD; and Centers Research (CR), incubate emerging ideas and talent in areas defined by the Lab's Strategic Centers. All seven components are discussed in detail in this plan.

In FY21, the LDRD program allocated $167M to 459 projects that incurred total costs of $160M. 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 FY21, the beginning-of-year reserve budget was approximately $9.77M, to which $2.00M was added mid-year, almost all of which was committed well before year-end.

LDRD Actual Costs at FY21 Year-end by Component

Exploratory Research
31%
Innovate at the frontiers of technical disciplines

Directed Research
43%
Create multidisciplinary solutions to complex problems defined by Lab strategy

Total LDRD Program
FY21: $160M

As of FY21 close.

Early Career Research
5%
Develop next-generation technical leaders

Postdoctoral R&D
5%
Attract and recruit top-quality talent into the Lab's pipeline

Mission Foundations
5%
Translate discovery into novel mission solutions

Centers
4%
Incubate emerging ideas and talent in areas defined by the Lab's Strategic Centers

Director's Initiative
7%
Invest in the Lab Agenda with the rigor and creativity of LDRD

Director's Initiatives

In FY21, LDRD funded 31 DI projects, investing 7% of the program's research funds.

LDRD Director's Initiatives are strategic efforts first implemented in FY19. The Initiatives focus on strategic objectives within the Laboratory Agenda. 20 of those projects started in FY21 and respond to eight Agenda objectives (see the figure below).

The senior Laboratory leaders responsible for each objective work with the LDRD Program Office and the Deputy Director for Science, Technology, and Engineering to identify strategic growth areas and potential projects. Director's Initiatives may be executed as either special projects or special calls. In either case, Director's Initiatives submit a proposal that is peer reviewed by independent reviewers, following criteria derived from the LDRD mission objectives. The duration of Director's Initiatives is between one and three years.

FY21 Laboratory Agenda Objectives Supported by LDRD Director's Initiatives

1.2/2.6
- Casting: Design Responsiveness and Rapid Qualification
- Welding: Design Responsiveness and Rapid Qualification
- Powder Materials: Design Responsiveness and Rapid Qualification
- An Investigation of Variables Affecting Plutonium Hydriding

1.3
- Flight Software Framework for Agile Response to Global Security Threats
- Artificial Intelligence (AI)-Driven Collection and Models for Trust/Reliability of Integrated Space Surveillance Data

1.4
- Enabling Design Agility in a Joint Test Assembly Flight Body

1.0 NUCLEAR SECURITY

Excellence in Nuclear Security

Design, produce, and certify current and future nuclear weapons and reduce global nuclear threats

1.1 Execute LANL's Manufacturing mission to deliver 30 plutonium pits per year
1.2 Transform nuclear weapons warhead design and production
1.3 Anticipate threats to global security; develop and deploy revolutionary tools to detect, deter, and respond
1.4 Support modernization of LANL warhead systems
1.5 Assess the stockpile as it ages and project weapon system lifetimes

2.0 MISSION-FOCUSED SCIENCE, TECHNOLOGY, AND ENGINEERING

Excellence in Mission-Focused Science, Technology, and Engineering

Deliver scientific discovery and technical breakthroughs that support DOE and NNSA missions

2.1 Refine and enhance the LANL capability pillar framework
2.2 Advance accelerator science, engineering, and technology to enable future stewardship capabilities
2.3 Advance the frontiers of computing to exascale and beyond
2.4 Assert leadership in the national quantum initiative
2.5 Develop and implement an integrated nuclear energy and nuclear materials initiative
2.6 Implement an integrated initiative for plutonium and actinide missions based on FY20 strategy
2.7 Implement a national security life sciences initiative

2.2
- Cryogenically Cooled Particle Accelerators for Transformative Improvement

2.4
- Molecular Framework Architectures for Quantum Information: Phase 1

2.5
- Data Driven Accelerated Fuel Qualification for Nuclear Fuels

2.6
- The Effect of Defects on the PuGa Phase Boundaries
- Enhancing Resonant Ultrasound Spectroscopy (RUS) to Measure the Elastic Properties of Complex Multi-Material Actinide Systems for In-Situ Applications
- Method for Extending the Plutonium-238 Supply
- Rapid Actinide Identification via Luminescence (RAIL) Sensor
- Influence of Defects on the alpha to beta Phase Transformation in Plutonium
- Corrosion Protection of Plutonium using Atomic Armor
- New Technique for Uranium Hydride Analysis using Ultracold Neutrons

2.7
- Global Trends, Resiliency, and Recovery
- Scalable digital biosurveillance to advance pandemic science and preparedness
- Biotechnology for Regional Climate Resilience

Directed Research

In FY21, LDRD funded 53 DR projects, investing 44% of the program's research funds.
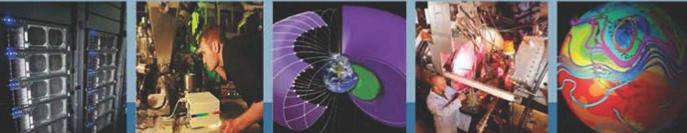
The DR component is LDRD's flagship investment and makes long-range investments in multidisciplinary projects in key competency or technology-development areas vital to LDRD's long-term ability to enable the Lab to execute its missions. DR projects are typically funded at up to $2M per year for three years.

Annual planning for DR directly ties to the Capability Pillars. Priorities within each Capability Pillar are set to maintain a balanced LDRD-DR portfolio in support of the Laboratory's capability goals. Priorities may include not just strategic capabilities, but also mission challenges requiring new and innovative approaches. Priority areas for each capability pillar (previously named "Focus Areas") are outlined below. Based on these priorities, staff submit proposals for peer review in a two-stage process.
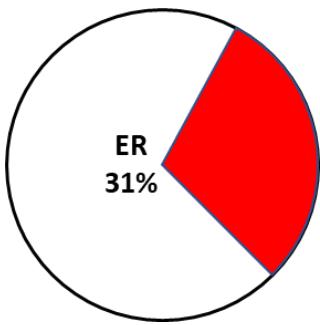
Note: Beginning with proposal calls released in FY21, LDRD fully incorporates the sixth Pillar, namely "Weapons Systems."

While the SIP is strongly aligned with respective Pillar strategies, the SIP has a narrower focus than that of the overall Pillars, due to considerations such as urgency of need, timeliness of opportunity, and LDRD-DR portfolio balance considerations. Further, the SIP is responsive to both internally perceived capability gaps and to emerging strategic directions identified by the National Nuclear Security Administration (NNSA) and Agency-specific strategies.

Exploratory Research

In FY21, LDRD funded 201 ER projects, investing 32% of the program's research funds. (These included 43 new starts based on the regular competitive call, with similar numbers continuing from FY19 and FY20, and the short-term projects discussed in the reserve section of this report.)

The ER component is focused on building technical staff competencies in key strategic disciplines that ready the Lab to address current and future national missions. Initiated by technical staff from across the Laboratory, ER projects explore highly innovative ideas in Technical Categories that underpin Laboratory missions (see below). ER projects are funded up to $360K per year for three years.
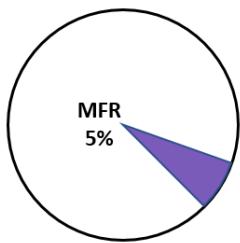
Exploratory Research is the most important channel for purely bottom-up creativity at the Laboratory. Division endorsements are not required for ER proposals; instead, this component of the program is operated as an open and competitive path for every staff member to pursue funding for his/her leading-edge idea. While some ER technical work may have a less direct tie to Laboratory missions, the technical capability underpinning the work must be directly relevant to one or more Laboratory missions.

Initiated by technical staff from across the Laboratory, ER projects explore highly innovative ideas in 10 Technical Categories that support Laboratory missions. Review teams for each Technical Category evaluate ER proposals. Distribution of funded ER projects across the Technical Categories is roughly uniform.

Technical Categories for Proposals Solicited in FY21

- *Advanced Materials Science and Engineering (AMSE)
- Atomic, Molecular, Quantum, and Optical Sciences (AMQOS)
- Biological Sciences (BIOS)
- Chemical Sciences (CHEM)
- Computational Methods and Computer Science (CMCS)
- Data Science and Mathematics (DSM)
- Earth and Space Sciences (ESS)
- Emergent Materials Behavior (EMB)
- High-Energy-Density Matter, Plasma, Fluids, and Beams (HPFB)
- Quarks to the Cosmos (QTC)

* Evolved to "Materials Processing, Structure, Properties, and Performance (MPSPP)" for proposals solicited during FY22.
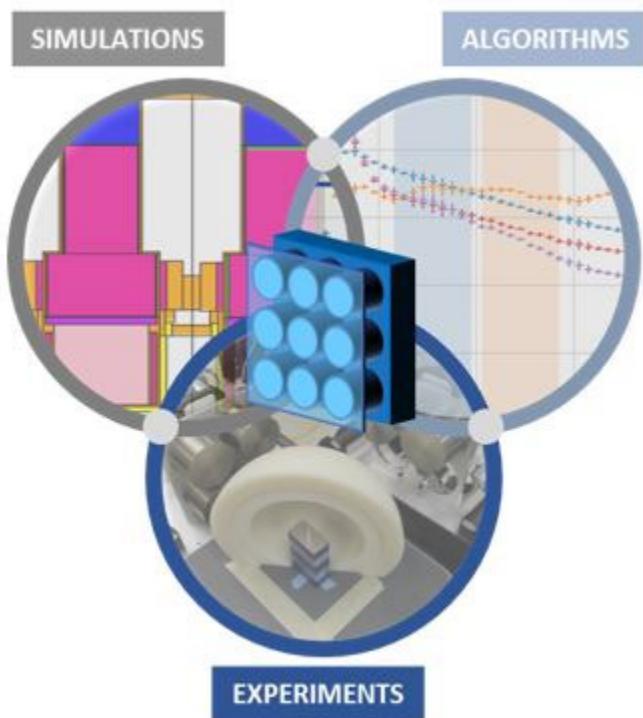
Mission Foundation Research

In FY21, LDRD funded 28 MFR projects, investing 5% of the program's research funds.

MFR is an intentional investment in applied science and engineering relevant to national security missions. The component was initiated in FY17 to address mission needs in the technology readiness level (TRL) 3-5 regime. Proposals must respond to "mission problem statements" reflective of mission needs across the Lab as defined in the Lab Agenda. MFR projects are initially funded at about $160K over 9 months (Phase 1), with additional funding awarded for those projects selected to continue into phase 2 (typically 16 months).

The LDRD Office organized an inaugural Mission Foundations Research (MFR) Connection event in September 2021. The MFR Connection was an opportunity not only to present the exciting results of the LDRD MFR portfolio, but also to provide a venue for technical staff, line management, and program management to discover and develop new collaborations and paths from LDRD to program. The event showcased ending Phase 2 MFR projects that started in FY20, with the goal of demonstrating how these projects have translated discovery into novel mission solutions of importance to national security missions. The results of these ending projects were presented in a "Science in 5" format, with a networking session for all event invitees to follow.

Figure: The nuclear emergency response mission requires understanding of any potential nuclear device. Its design must be understood. Theresa Cutler's (NEN-2) MFR project – "Neutron Spectroscopy (NS) for Nuclear Emergency Response (NER) Applications" – makes use of neutron spectroscopy in this effort. The project started in FY21 and was one of ten projects selected to continue into Phase 2 through FY22. A successful Phase 2 study will result in a proof-of-concept, potentially field-able, detector system with experimental results from NER-like items. This prototype will demonstrate the benefits of capitalizing on the information-rich neutron energy information using full NS unfolding, which in turn can provide reliable actionable information to determine follow-on procedures for NER applications.

FY21 Mission Foundation Research Projects

Accelerators: Materials and methods for LANL accelerator facilities, projects, and future high performance accelerators

Study for Alternative Cavity wall and Inductive Insert Material	Charles Taylor (AOT-AE)
A Novel Heater Wire to Improve H- Ion Source Filament Lifetime	Prabir Roy (AOT-AE)
*Solution fabricated solid-state X-ray imager	Wanyi Nie (MPA-CINT)
*High -Performance/-Precision/-Z (HPPZ) Scintillator Grids via Advanced Electrochemistry	Enkeleda Dervishi-Whetham (SIGMA-2)

Weapons Production: Agile and Efficient Nuclear Manufacturing

*Implementing a Novel Ultrasonic Filtration Technology to Eliminate Hydroxide Precipitation Bottlenecks at TA-55	James Coons (C-CDE)
*Agile System for Electrochemical Dissolution of Bulk Actinide Oxides	Benjamin Karmiol (AMPP-4)
*On-machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication	Wendel Brown (PT-2)

Energy Security: machine learning and molten salt reactors

*Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches	Youzuo Lin (EES-17)
Exploring Safeguard Signatures with Energy Resolved Neutron Imaging for Future Molten Salt Reactor Designs	Alexander Long (MST-8)
Learning Fault Physics and Failure in Hydraulic Injection	Paul Johnson (EES-17)
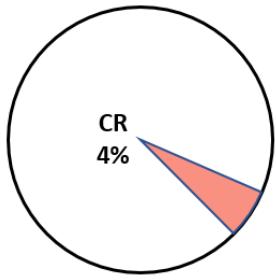
Weapons Engineering: Nuclear explosive package

*Modern Radiation Case Material for an Agile Complex	Kendall Hollis (SIGMA-1)
*Megavolt generator for multiple-pulse hydrotesting	Nicola Winch (NEN-2)
*Computational Modeling Tool for Rapid Performance Characterization of Novel High-explosive Design Geometries	Von Whitley (XTD-SS)

Global Security: Nuclear emergency response

*Neutron Spectroscopy for NER Applications	Theresa Cutler (NEN-2)
Intelligent Coupling of X-ray Radiography and Acoustics for Accurate Rapid Assessments for Emergency Response	John Greenhall (MPA-11)
Detector Response Toolkit for Nuclear Emergency Response	Madison Andrews (XCP-7)

*Indicates project that have continued to Phase 2

Centers Research

In FY21, LDRD funded 9 CR projects, investing 4% of the program's research funds.
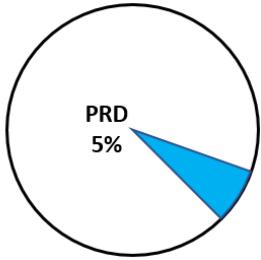
To infuse new ideas and people into the Laboratory, LDRD has made a commitment to partner with the Lab's "Strategic Centers." The CR component is focused on developing the nation's next-generation workforce and leadership talent and to serving as an incubator for the introduction of emerging ST&E into DOE and NNSA missions. CR projects are typically funded up to three years and single-year per-project funding in FY21 ranges from approximately $750K-$1,900K.

The Centers are organized under the National Security Education Center (NSEC), which supports a broad spectrum of interdisciplinary science that underpins the Lab's mission in national security. Collaborations established through the Centers provide Lab programs with new ideas, people, and contacts both inside and outside the Lab. For example, collaborative work with universities fosters top-quality research at the Lab in the more basic or fundamental aspects of fields that map into existing and/or emerging mission areas of the Laboratory. The Centers also introduce students and postdocs to the scientific interests of the Laboratory. The Centers nucleate new research areas at the interface between emerging frontiers in the scientific community and the Laboratory's national security mission and are instrumental in anticipating future needs.

LDRD funds the Centers Rapid Response research and development program that supports short-term, rapid-turnaround high-risk ideas or feasibility studies. Three of the Centers have formal postdoctoral programs funded through LDRD, targeting strategic areas where new staff members are recruited at the PhD level.

Former Seaborg postdoctoral fellow Dr. Sarah Hernandez, partially funded by LDRD, performs actinide research in the Nuclear Materials Science (MST-16) group. Consistently, over half the postdocs at the Laboratory are funded at least 10% by LDRD. In FY21, Hernandez was the principal investigator on a LDRD Director's Initiative, "Influence of Defects on the alpha to beta Phase Transformation in Plutonium." The project was selected as part of LDRD and Seaborg Institute joint proposal call.

Postdoctoral Research and Development

In FY21, LDRD funded 84 PRD projects, investing 5% of the program's research funds.

The PRD component of the LDRD program ensures the vitality of the Laboratory by recruiting early career researchers. Through this component, LDRD funds Postdoctoral Fellows to work under the mentorship of PIs on highly innovative projects.
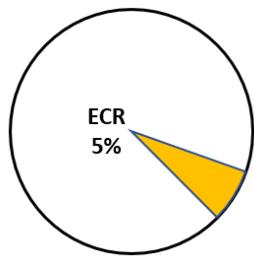
PRD projects are funded under two appointment types intended to represent the most promising among the Laboratory postdoc population–Director's Postdoctoral Fellows and Distinguished Postdoctoral Fellows. Distinguished Fellows are supported at a higher salary and show evidence of providing a new approach or insight to a major problem that will likely have a major impact in their research field. To recognize their role as future science and technology leaders, Distinguished Fellows are named after some of the greatest leaders of the Laboratory's past, such as Los Alamos Medal laureate Darleane Christian Hoffman.

In FY21, LDRD supported 72 Director's (2 years, extendable to 3) and 11 Distinguished (3 years) Fellows. The LDRD program encourages conversion to staff by allowing the new staff member to continue the PRD project until its originally planned end date.

LDRD also encourages collaboration between postdocs and Laboratory staff. More postdocs are hired through DR and ER projects than directly through PRD appointments. Counting both avenues, the LDRD program supported 59% of the 665 postdocs employed at the Laboratory for at least part of FY21.

Postdoctoral researchers are an important part of the Los Alamos pipeline and are often drawn in by the opportunity to work with LDRD. Pictured here is Sophie Couslon, a LDRD Director's Postdoctoral Fellow at Los Alamos. Her research focuses on flow and deformation in the Earth's interior and the effect these processes have on changing sea level and ice sheet stability. She received her Ph.D. at Harvard University where she initiated the work she is currently working on via LDRD project, "Climate Change-induced Seismicity? Quantifying the Impact of Ice and Ocean Loading on Crustal Stress and Seismicity in the Russian Arctic" (20210952PRD3). [Read more in the Harvard Gazette](#) or in this article in [Nature](#).
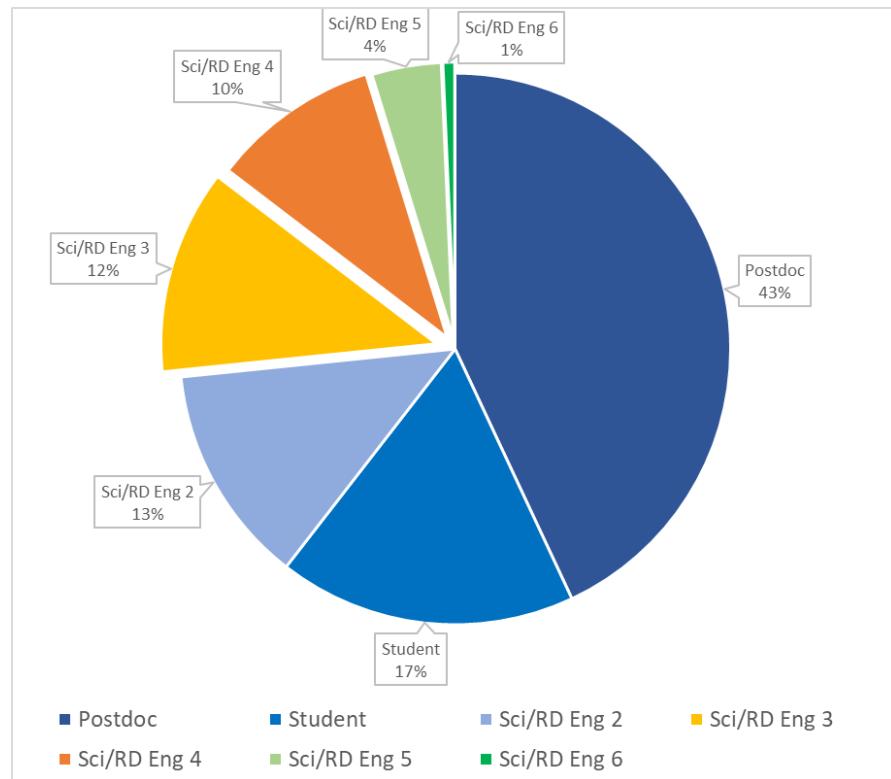
Early Career Research

In FY21, LDRD funded 53 ECR projects, investing 5% of the program's research funds.

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 support the development of early career researchers, aiding in the transition from postdoc or student to full-time staff member, and to stimulate research in disciplines supported by the LDRD program. ECR projects are funded up to $230K per year for two years. The number of ECR new starts tracks with the Laboratory's hiring rate, which has been steadily high in recent years.

Early Career Research PIs must have received their highest degree within the last 10 years and been hired as a Laboratory technical staff member no more than three years prior to the call. Individuals with limited-term appointments are eligible; however, an Associate Level Directorate endorsement confirming the organization's intent that the proposer will make a long-term contribution to the Laboratory must be submitted to LDRD.

LDRD Invests Heavily in Early Career Staff Across All Components

Hours charged to LDRD Projects
In a recent analysis, LDRD found early career researchers (in this case defined as postdocs, students, and Scientist/R&D Engineer 2) contribute the majority of hours to LDRD projects. Early Career and Postdoctoral projects are just a fraction of this early career support. LDRD is essential to retaining this critical demographic. (Data current though FY19.)
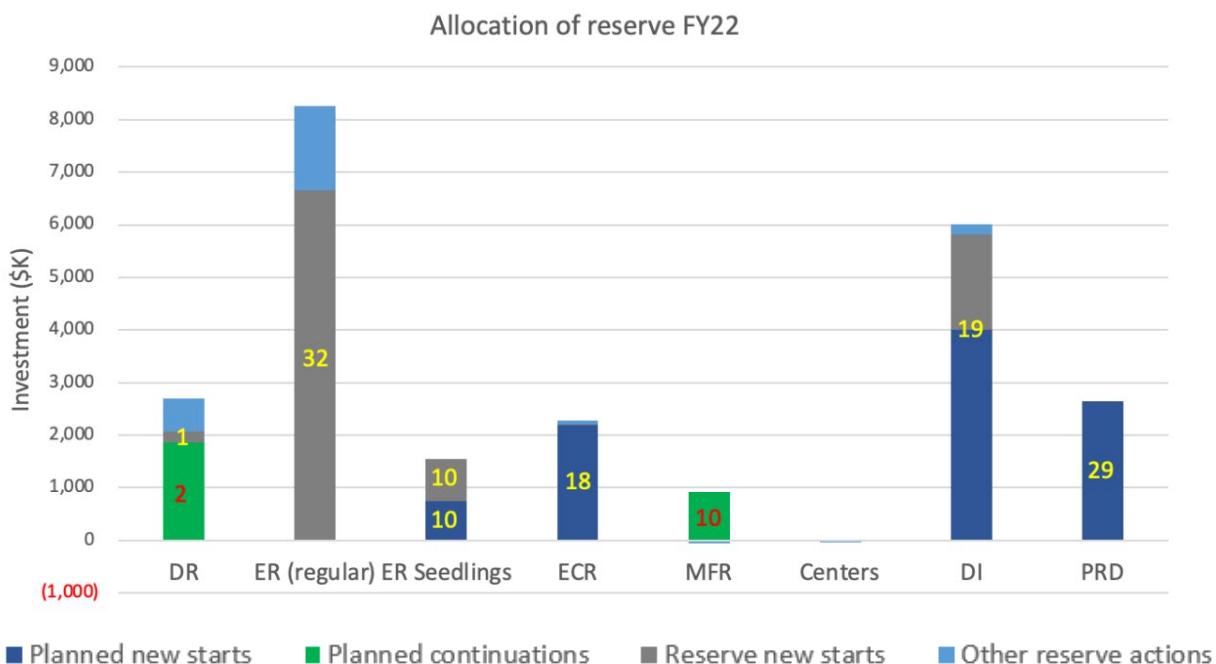
Not all of the LDRD budget is allocated to individual projects at the beginning of the fiscal year. Some is set aside for planned new starts based on calls for the PRD, ECR, DI, and MFR components; and some is unencumbered, available for timely opportunities as the year unrolls. At the beginning of FY21, the unencumbered reserve was $9.77M, to which $2.00M was added mid-year. In addition, $12.37M was set aside for new projects in delineated areas, most of which would be selected via open calls (and all approved via peer review), as follows:

Component	Set aside	# of projects
DR full project continuations post feasibility review	$1.86 M	2
ER Seedling new starts	$0.75 M	10
Early Career new starts	$2.20 M	18
Mission Foundations Phase 2 continuations	$0.91 M	10
Director's Initiative new starts	$4.00 M	TBD
Postdoc project new starts	$2.65M	TBD

The LDRD Program Office improved the process for tracking reserve funding in FY20 and used the same methods in FY21. Based on this tracking, the figure below shows how the set asides and unencumbered reserve were allocated.

Allocation of planned set asides and unencumbered reserve for FY21. The numbers in yellow show the number of new start projects initiated after the beginning of the fiscal year, while the figures in red show project continuations.
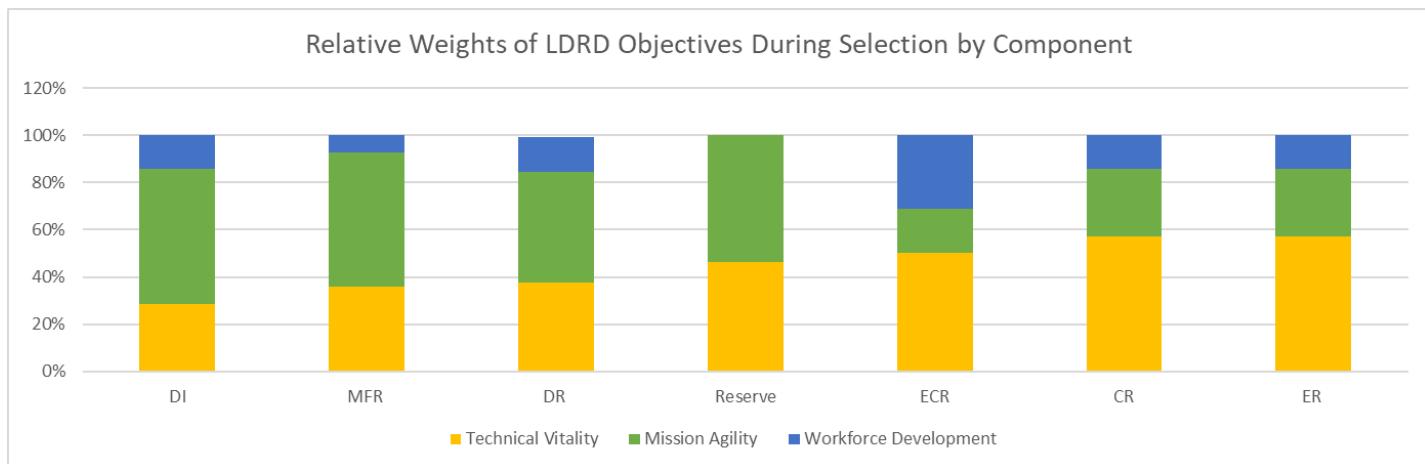
The set asides for Early Career and postdoctoral (PRD) projects were executed essentially as planned, as were the DR project continuations (both projects passed their feasibility reviews with flying colors), and the MFR continuations into Phase 2, which were based on peer review of the Phase 1 results and Phase 2 proposals. The response to the ER Seedling call was unexpectedly strong, so LDRD funded not only the planned 10 starts, but drew from reserve for another 10 starts. Most of the unencumbered reserve was invested in ALD-nominated proposals which were then peer reviewed. Those that passed peer review were prioritized for funding, resulting in new starts of 1 short-term DR project and 32 ER projects. The same prioritization process yielded budget increases to existing projects, as shown in light blue in the figure.

Finally, ALD response to the needs of the Laboratory agenda was strong, so that the commitment to new Director's Initiatives was increased from $4M to $6M, again drawing on the unencumbered reserve.

LDRD Objectives Across the Portfolio

LDRD strives for a portfolio that reflects all three LDRD objectives–Technical Vitality, Mission Agility, and Workforce Development. The balance between technical vitality and mission relevance has evolved over the last few years; and, considering the whole LDRD portfolio, mission relevance has a bit more weight than previous years. LDRD has also added explicit consideration of workforce development to proposal and appraisal criteria.

The LDRD Program Office puts thoughtful consideration into how the weighting of selection criteria for each component addresses the three LDRD objectives. The scoring matrix for each component states how the criteria are weighted.

Shown here is the share of selection criteria for each of the LDRD objectives for each LDRD component. The several components form an integrated portfolio that balances the objectives. The purpose of mapping the criteria to the objectives is to ensure both proposers and reviewers remain focused not only on an individual project, but also on how the project benefits the Laboratory and the Nation. Note: Data is current as of 7/22/21 and reflects criteria for projects selected in FY21.

Program Value

Congress established the Laboratory Directed Research and Development (LDRD) program at the Department of Energy (DOE) national laboratories in 1991 to foster excellence in science and technology and to ensure the laboratories are technically vital and prepared to meet today's needs and tomorrow's challenges. LDRD achieves this by supporting high-risk, potentially high-payoff research and development. At Los Alamos, the LDRD program provides the most significant resource for internally directed scientific and technical investments.

The LDRD program is a key resource for addressing the science and technology goals of the Laboratory, as well as enhancing the scientific capabilities of Laboratory staff. Through careful investment of LDRD funds, the Laboratory builds its reputation, recruits and retains excellent scientists and engineers, and prepares to meet evolving national needs.

The programs' objectives are clear and crucial: Technical Vitality, Mission Agility, and Workforce Development.

FY 2021 LDRD Program at-a-glance

$160M
Total Program Cost

459
Total Number LDRD Projects

201
New LDRD Projects in 2021
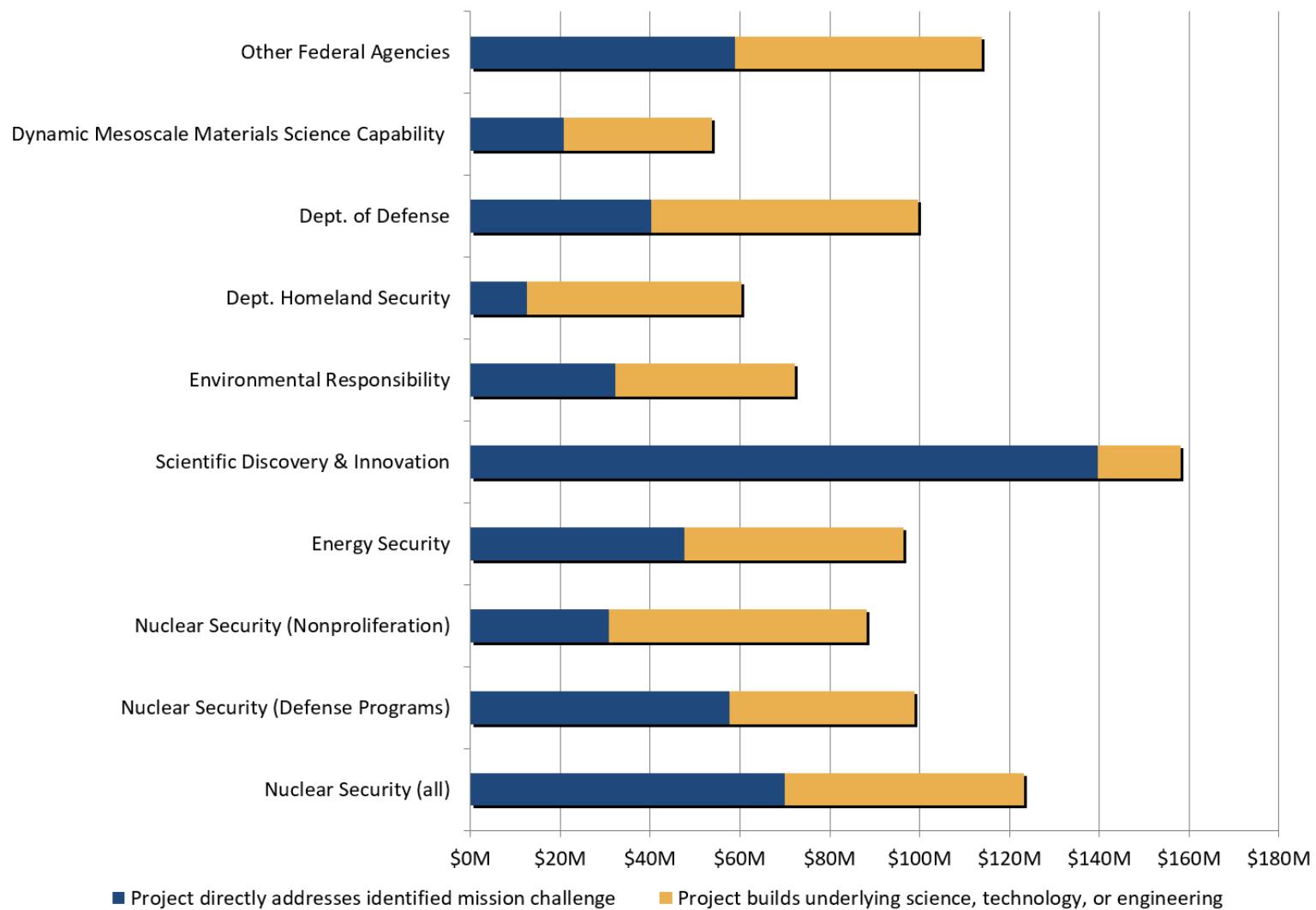
LDRD-supported Postdocs	**59%**	391 of 665 postdocs at Los Alamos
LDRD-supported Postdoc to Staff Conversions	**54%**	44 of 81 conversions at Los Alamos
Peer-reviewed Publications	**38%**	830 of 2,207 publications at Los Alamos
U.S. Patents Issued	**30%**	14 of 46 patents at Los Alamos
R&D 100 Awards	**57%**	4 of 7 R&D 100 awards at Los Alamos

Although LDRD costs are only a small portion of the Laboratory's base (6%), LDRD yields well over its share of postdoc conversions, publications, patents, and technical awards.

3/17/2022
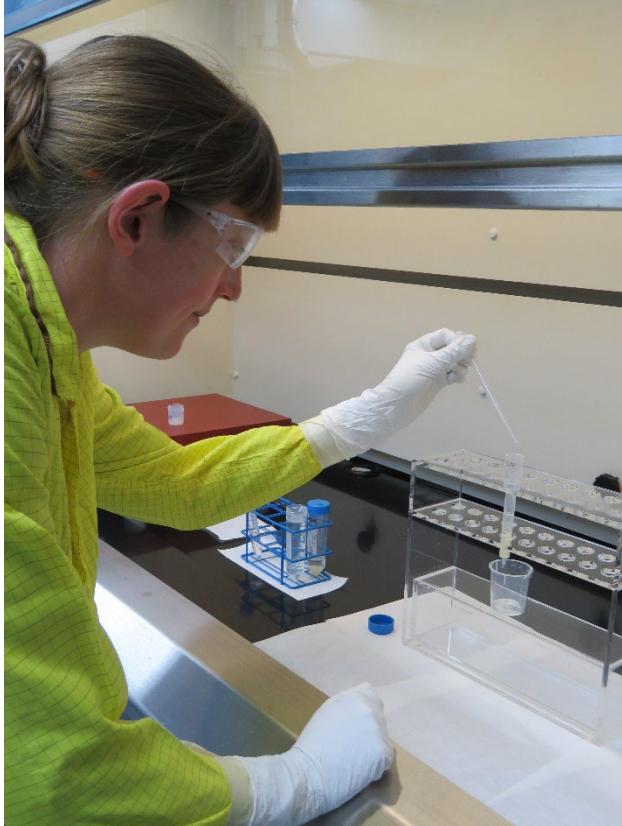
Mission Relevance

Mission relevance is one of the most important criteria in the evaluation of the LDRD program, as well as 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 and 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.

Mission Impact of FY21 LDRD Portfolio ($M)

First and foremost, Los Alamos LDRD projects are required to address one or more of the DOE or NNSA mission areas. The sum of the total LDRD investment in relevant missions is far greater than the annual LDRD budget; investment in one project often contributes to and impacts multiple missions.

Due to the basic science nature of LDRD, the work often proves relevant to several missions and agencies. LDRD data sheets include an analysis of mission relevance in which the PI indicates direct, underlying and clearly related, or no relevance to federal agency missions, nuclear security and national defense, energy security, environmental stewardship, and areas of scientific discovery and innovation.

Due to the basic science nature of most LDRD projects, the work often proves relevant to several missions and agencies. For example, researcher Joanna Denton (pictured left) worked to add parent-granddaughter radiochronometry to the Lab's nuclear forensics toolbox, enabling the age of a material to become more tightly constrained. The age of a material, obtained through radiochronometry, is a key predictive signature in a nuclear forensics investigation with significant implications for global security missions like nuclear nonproliferation, counterproliferation, and counter terrorism. Furthermore, Denton's work has important implications for the field of chemical science. (1/15/19-1/14/22)

Project Appraisals

The LDRD Program Office oversees formal appraisals of all second- and third-year projects (not including PRDs). A primary objective of the project appraisals is to assess progress and provide peer input to help PIs maintain the highest quality of work possible. The appraisals also help the LDRD Program Office monitor and manage the program portfolio.

LDRD formal project appraisals in FY21 indicate a high level of productivity and excellence. The LDRD Program Director oversees the Exploratory Research (ER) appraisals in collaboration with the technical divisions. Projects were appraised according to criteria that map to the LDRD objectives: technical vitality, mission agility, workforce development, as well as a fourth criteria, namely, project execution. As of this report, 86 appraisals have been conducted and scores are currently available for 85 projects. The LDRD Program Director's overall impression of a high level of productivity and excellence) is upheld by the appraisal scores, in which the weighted average is 4.37 ("excellent" on the standardized scoring theme).

Directed research appraisals conducted in FY21 demonstrated a similar high level of productivity and excellence. DR projects are appraised every year of the project, with a half-day appraisal at the beginning of year 2, a shorter appraisal at the beginning of year 3, and a final appraisal after the project ends. 14 year 2 appraisals were conducted, with an average score of 4.4 (or "excellent"). The average score rose to the "outstanding/excellent" range for the 13 year 3 appraisals (4.6), pointing to the efficacy of the appraisal process to help PIs maintain high quality work. Final appraisals were conducted for 11 DR projects, with an average score of 4.5.

Those few appraisals that are significantly less than "excellent" result in discussions with the project and line leadership, and, when needed, corrective action plans.

In addition to the formal project appraisals, LDRD regularly holds informal project visits, paying particular attention to reserve projects, projects just getting started, and projects in their last few months. The objective is to understand project accomplishments and any opportunities for improvement to the project or the LDRD program. A project visit takes the LDRD Program Director or Deputy into the field, typically to the PI's office or lab but this year into a WebEx conference, for a discussion of up to 90 minutes.

Performance Indicators: LDRD at LANL

This section presents both short and long-term performance indicators LDRD maintains to evaluate the success of LDRD projects and to inform planning activities at the Laboratory. Although LDRD costs are only a small portion of the Laboratory's base (6%), LDRD yields well over its share of intellectual property, postdoc conversions, publications, patents, and technical awards.

Intellectual Property

An indication of the cutting-edge nature of research funded by LDRD is the contribution the program makes to the Laboratory's intellectual property. Year after year, projects sponsored by LDRD achieve a disproportionately large percentage of the patents and copyrights issued for Los Alamos research.

U.S. Patents

Number of US patents issued in a given FY
LDRD supported: Patents issued that would not exist if not for initial work funded by LDRD

	FY17	FY18	FY19	FY20	FY21
LANL U.S. patents	43	51	53	46	46
LDRD supported	9	10	20	19	14
% due to LDRD	21%	20%	38%	41%	30%

Software Copyrights

Number of software copyrights created in a given FY
LDRD supported: Software copyrights issued that would not exist if not for initial work funded by LDRD

	FY17	FY18	FY19	FY20	FY21
LANL software copyrights	148	113	147	119	120
LDRD supported	21	19	16	39	48
% due to LDRD	14%	17%	11%	33%	40%

Note: The majority of copyrights granted at LANL are software copyrights. Developing and exchanging software is a critical stepping stone in the collaborative efforts which drive the success of many projects. LANL has three primary software release types: open source (unrestricted release of source code via a publicly available repository); commercial/noncommercial licensing (controlled release of code to commercial entities, academic collaborators, or foreign government agencies); and government use only (controlled release of code to U.S. government agencies/contractors).

Invention Disclosures

Number of declarations and initial records of an invention (a new device, method, or process developed from study and experimentation)

LDRD supported: Disclosures issued that would not exist if not for initial work funded by LDRD

	FY17	FY18	FY19	FY20	FY21
LANL disclosures	117	109	118	115	101
LDRD supported	24	40	39	34	33
% due to LDRD	21%	37%	33%	30%	33%

Tech Snapshots

Los Alamos has identified a broad range of technologies that could enhance an existing product, define a new product, or launch a start-up. Our technologies have the potential to give your company a competitive edge in the market. Each are at different stages of development some ready to license and others looking for a partner to help mature into a disruptive application. Check out the Technology Snapshot platform to explore the wide variety of technologies available.

Search for... Search

Advanced Materials   Biology   Chemistry   Cyber Security

Data Analytics   Earth and Environmental   Infrastructure   Manufacturing

Nuclear   Sensors   Software   Space

"Tech Snapshots" on many of these technologies can be found on the Richard P. Feynman Center for Innovation web site.

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 FY21, 38% of LANL peer-reviewed publications have roots in LDRD. The quality of these publications is evidenced by the frequency they were cited, where the LDRD percentage (45% in FY21) has been rising in recent years.

Publications

Number of peer-reviewed publications
LDRD supported: Publications for which LDRD made a substantial contribution

	FY17	FY18	FY19	FY20	FY21
LANL publications	2,001*	2,100	2,066	1,971	2,207
LDRD supported	525*	613	714	678	830
% due to LDRD	26%	29%	35%	34%	38%

*FY17 data corrected 3/12/20. Percentage LDRD did not change.
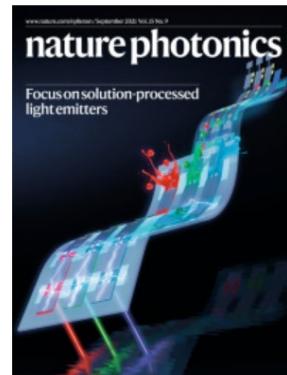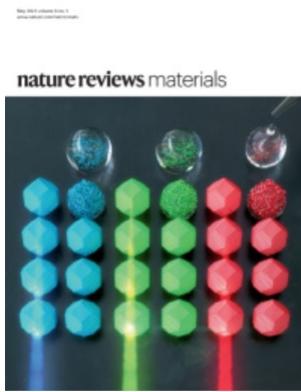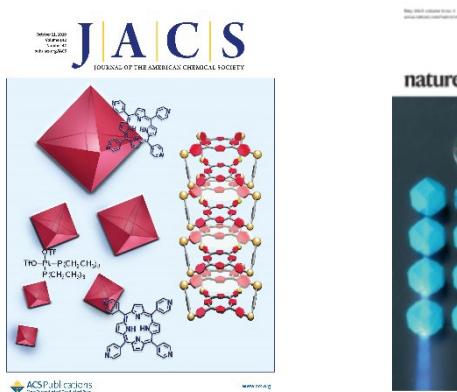
Citations

Number of citations of peer-reviewed publications
LDRD supported: Citations of publications for which LDRD made a substantial contribution

	FY17	FY18	FY19	FY20	FY21
LANL citations	42,815	29,161	16,565	26,519	6,006
LDRD supported	15,717	11,149	7,552	12,327	2,726
% due to LDRD	37%	38%	46%	46%	45%

Note: Citations are current as of 2/17/22 and drawn from Web of Science–a website that provides access to multiple databases that provide comprehensive citation data for many different academic disciplines. Originally produced by the Institute for Scientific Information, it is currently maintained by Clarivate Analytics.

LDRD work led by researcher Victor Klimov (20200213DR, 20210176ER) was featured in FY21 on three journal covers, namely: Journal of the American Chemical Society (Left), nature Review Materials (Center), and Nature Photonics (Right).

Broad Intellectual Engagement

External collaborations are essential to the conduct of research and development in LDRD. By working with other national laboratories, academia, and industry, LDRD investigators access leading facilities and knowledge in the U.S. and abroad.
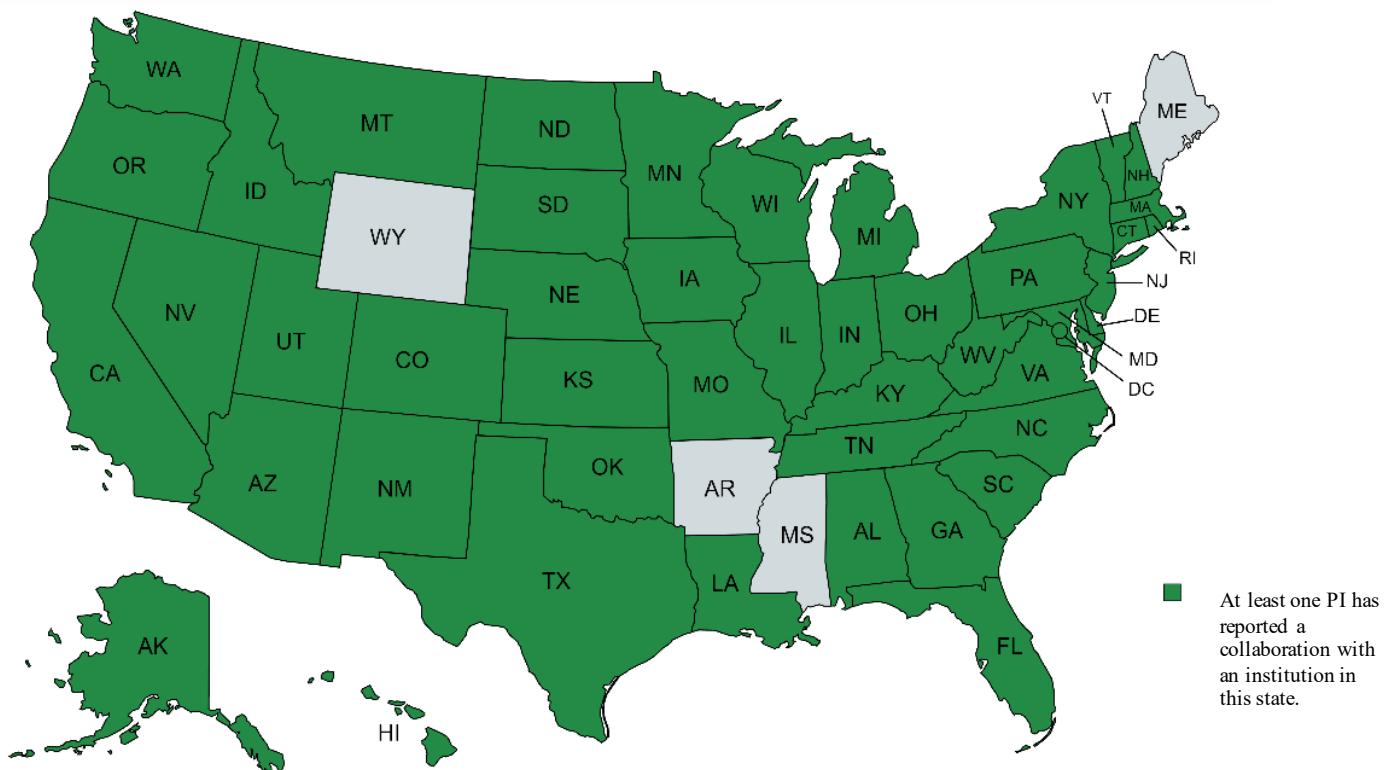
Collaborating with universities is a great way to leverage external expertise and can help feed the pipeline through which the Laboratory recruits postdocs and students. Subcontracts with universities that fund postdocs and sometimes other faculty are fairly common in LDRD.

That said, most external collaborations under LDRD are on a no-exchange-of-funds basis, where collaborators each use their own funding and collaborate for the mutual benefit of working together. Such collaborations are broadly encouraged, subject only to Laboratory policies such as export control and intellectual property management. LDRD researchers self-report these no-exchange-of-funds external collaborations. Because they are no-exchange-of-funds, these collaborations demonstrate the value that collaborators find in partnering with LDRD work solely on the basis of its scientific/engineering merit.

In FY20 and FY21, LDRD researchers reported 1,685 external collaboration, including 1,294 collaborations with US scientists and engineers and 391 with foreign collaborators.

Note: A collaborator is defined as a likely co-author on a proposal, patent, or publication (including formal internal reports) as a result of the project and someone with whom the reporting PI is in direct contact with.

Recent LDRD external collaborators within the United States come from 46 states and Washington DC. (Data from FY20 and FY21.)

At least one PI has reported a collaboration with an institution in this state.

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. LDRD is also instrumental in retaining new talent from the student and postdoc pool at the Laboratory.

Postdoctoral Researcher Support
Number of postdoctoral researchers working full- or part-time for the Laboratory
LDRD supported: Postdoctoral researchers charging at least 10% time to LDRD

	FY17	FY18	FY19	FY20	FY21
LANL Postdocs	497	556	632	655	665
LDRD supported >10%	263	281	376	363	391
% due to LDRD	53%	51%	59%	55%	59%

Note: Includes data on postdocs in FY21 from Sept. 29, 2020 to Sept. 26, 2021.

Postdoctoral Researcher Conversions
Number of conversions from postdoctoral researcher to a member of the staff
LDRD supported: Conversion of postdoctoral researchers who charged at least 10% time to LDRD in the fiscal year preceding the conversion

	FY17	FY18	FY19	FY20	FY21
LANL Conversions	69	81	87	75	81
LDRD supported >10%	37	37	39	35	44
% due to LDRD	54%	46%	45%	47%	54%

Note: Includes data on postdocs in FY21 from Sept. 29, 2020 to Sept. 26, 2021.

Students
There are many opportunities for students to play important supporting roles on LDRD projects. A student may serve as a Co-Investigator on any LDRD proposal. For example, it is common to see students funded on ER and DR projects. There are also opportunities for a student to work with an early career staff member on an Early Career Research project, where the early career staff member would serve as the PI and the student would serve a significant secondary role to that PI. Furthermore, the Centers have specific calls for student projects.

> In FY21, 333 students worked at least 40 hours on LDRD projects. This compares to 258 students in FY20.

The LDRD program is an investment in the nation's future, ensuring mission support that is often realized after many years. This section highlights the longer-term (>5 year) impact of LDRD as a national asset. These performance indicators will be updated annually. As it is expected that the data may vary from year to year, long-term running totals will also be included and updated every 5 years.

Background
As part of a commitment to continuous improvement, representatives from each LDRD program at the NNSA laboratories regularly participate in a working group to share best practices and discuss strategies for tracking the long-term impact of LDRD investments. In FY20, the working group finalized a combination of common quantitative and qualitative long-term indicators, emphasizing a systematic approach. Additionally, the working group recognized that individual laboratories may choose to report other long-term indicators that fit their unique missions and capabilities.

Alignment with LDRD Objectives
The collective selection of indicators (both numerical and qualitative) illustrate the long-term payoffs/success of LDRD, with respect to all three LDRD objectives (Technical Vitality, Mission Agility, Workforce Development). Because indicators crosscut objectives, there is not an intent to provide a 1:1 mapping of indicators with objectives.
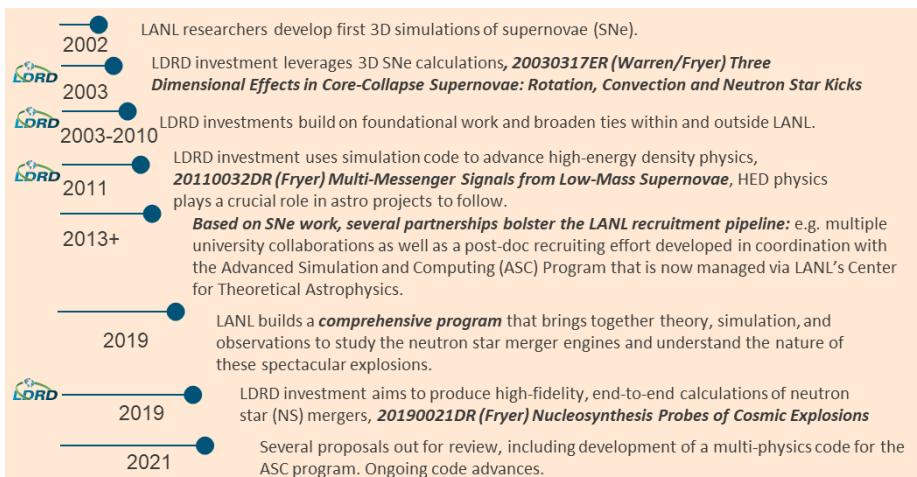
Importance of Qualitative Data
The difficulty of developing numerical indicators for success in R&D programs is widely recognized. The metrics working group was able to develop numerical success indicators for both Technical Vitality and Workforce Development. "Success stories" were found to be more flexible to capture the successes in Mission Agility, as well as aspects of the other two LDRD objectives that are not well-capture by numerical metrics.

Tracing impact back to LDRD
Throughout this section, you will see references to "LDRD roots." There is often a lot of discussion with PIs about what it means for an accomplishment to have "LDRD roots." A simple case would be if an idea for an invention arises during an LDRD project and work on the invention is completed during the period of LDRD investment. But R&D often does not advance on such a short timescale. In general, an accomplishment (invention, paper, capability, etc.) is determined to have LDRD roots if there are one or more LDRD projects without which the accomplishment would never have come into being. In other words, if one can identify an LDRD project that was critical to the accomplishment, then it is considered to have "roots" in that LDRD project. Other relevant definitions for the metrics shared are included in the sections to follow.

__Long-Term Success:__ By leveraging LANL physics and computational expertise, LDRD researchers diagnose the details of supernova explosions and probe the extreme physics behind them. Decades of LDRD investments in this area have results in many applications to nuclear security.

2002 — LANL researchers develop first 3D simulations of supernovae (SNe).

2003 — LDRD investment leverages 3D SNe calculations, *20030317ER (Warren/Fryer) Three Dimensional Effects in Core-Collapse Supernovae: Rotation, Convection and Neutron Star Kicks*

2003-2010 — LDRD investments build on foundational work and broaden ties within and outside LANL.

2011 — LDRD investment uses simulation code to advance high-energy density physics, *20110032DR (Fryer) Multi-Messenger Signals from Low-Mass Supernovae*, HED physics plays a crucial role in astro projects to follow.

2013+ — *Based on SNe work, several partnerships bolster the LANL recruitment pipeline:* e.g. multiple university collaborations as well as a post-doc recruiting effort developed in coordination with the Advanced Simulation and Computing (ASC) Program that is now managed via LANL's Center for Theoretical Astrophysics.

2019 — LANL builds a *comprehensive program* that brings together theory, simulation, and observations to study the neutron star merger engines and understand the nature of these spectacular explosions.

2019 — LDRD investment aims to produce high-fidelity, end-to-end calculations of neutron star (NS) mergers, *20190021DR (Fryer) Nucleosynthesis Probes of Cosmic Explosions*

2021 — Several proposals out for review, including development of a multi-physics code for the ASC program. Ongoing code advances.

Long-term Indicators

Professional Fellows (American Physical Society)
One relevant indicator of advancement and leadership in a ST&E field is the election of individuals as fellows of professional societies. This indicator reflects success for both the individual researcher and the laboratory as a whole. American Physical Society (APS) Fellows were selected as the exemplar due to the important linkage of physicists with NNSA's core stockpile stewardship mission. Furthermore, APS Fellowship is awarded based on scientific merit and impact over an extended period of time. (In contrast, some professional societies may also award fellow status based on service to the society.)

In FY20, five of the six LANL APS Fellowships were awarded to researchers with roots in LDRD. While there is sometimes minor fluctuation from year to year, multi-year analyses consistently reflect a high majority of APS Fellows with prior LDRD experience. At LANL, 65 of the 71 researchers who have been awarded APS fellowships since FY11 have prior experience with LDRD.

History of APS Fellows at Los Alamos National Laboratory

	Single-Year Statistics			Multi-Year Statistics		
	FY19	**FY20**	**FY21**	**FY11-15 (5 years)**	**FY16-20 (5 years)**	**FY11-21* (11 years)**
Total awards	5	6	3	38	30	71
Awards with LDRD roots	4	5	2	35	28	65
% with LDRD roots	80%	83%	67%	92%	93%	92%
Average years from first LDRD experience	10.00	12.20	15.00	8.94	11.82	10.41

*Initial year to date: Each Laboratory has chosen the appropriate lookback period that will ensure data integrity.

Why this matters
The fact that so many APS Fellows at the Laboratory have prior LDRD experience is a testament to LDRD nurturing their careers (workforce development) and the technical vitality of the Laboratory. LDRD draws high caliber talent into the Laboratory and considers the commitment to continue to develop these researchers to be crucial to the future success of both those researchers and the Laboratory.

"Recognition of their accomplishments by the American Physical Society demonstrates the vibrant engagement that the Laboratory's physicists have with the external scientific community and their contributions to physics research." – John Sarrao, Deputy Director for Science, Technology & Engineering

LANL Researchers Elected 2021 APS Fellows Have LDRD Experience

Three LANL scientists were elected Fellows of the American Physical Society (APS). Eric Brown, Nathan Moody, and Takeyasu Ito were chosen for their "exceptional contributions to the physics enterprise." Notably, Takeyasu Ito and Nathan Moody Have received recent LDRD funding, and Eric Brown is an active participant in LDRD peer review and other processes. Fewer than one half of one percent of APS members are elected as fellows each year.

From left: 2021 APS Fellows Eric Brown, Nathan Moody, and Takeyasu Ito.

Eric Brown was named fellow for technical leadership in the physics of materials at high pressures and strain rates, for technical advances in the understanding of the mechanical behavior of polymers, and for sustained leadership and service to the American Physical Society and the shock physics community. He is currently a senior scientist in the Office of Experiment Science. Brown served on the Strategy Team in 2017-2019 to help assess proposals for LDRD's flagship component Directed Research.

Nathan Moody was selected for fundamental developments in material physics methods to protect and enhance the ruggedness and performance of photocathodes and materials surfaces critical to particle accelerators. Moody is a technical staff member and group leader of the Applied Electrodynamics group within Accelerator Operations and Technology division at the Laboratory. He stewards Los Alamos' largest concentration of accelerator science, technology, and engineering talent and capability at the Laboratory. His work with LDRD began in 2007 when he was a principal investigator on an Exploratory Research project.

Takeyasu Ito was selected as an APS fellow for fundamental studies that led to the development of the world's most powerful ultracold neutron source, for its commissioning, and for its application to precision measurement of the neutron and its decay. Ito joined the Physics division at Los Alamos as a staff scientist in 2005. His work has focused on using ultracold neutrons as a probe for studying the consistency of the standard model of particle physics and searching for what may lie beyond it. His work with LDRD began in 2005 when he was an investigator on a Directed Research project.

R&D 100 Awards

Another relevant indicator of advancement and leadership in a ST&E field is R&D 100 Awards. The prestigious "Oscars of Invention" honor the latest and best innovations and identify the top technology products of the past year. The LDRD Program offices at each site often partner with sister organizations, such as the Intellectual Property Office and Public Affairs, to track whether R&D 100 winners (whether in the standard category or special awards) have "LDRD roots." Because of the long development time from idea (LDRD) to practical implementation (R&D100 Award candidate) the staff who work on something that wins an R&D 100 Award may not be the same staff who worked on the original R&D. Each site's LDRD Program Offices engage in an extensive interview process to uncover the details of how the LDRD work led to the celebrated invention.

In FY21, four of the seven R&D100 Awards received by LANL have roots in LDRD. While there is sometimes minor fluctuation from year to year, multi-year analyses consistently reflect a high majority of R&D100 winners with prior LDRD experience. At LANL, 36 of the 60 R&D100 awards given to LANL since FY11 have roots in LDRD. On average, awardees in 2021 with LDRD support trace the initial LDRD investment to three years prior.

History of R&D 100 Awards at Los Alamos National Laboratory

	Single-Year Statistics			Multi-Year Statistics		
	FY19	FY20	FY21	FY11-15 (5 years)	FY16-20 (5 years)	FY11-21* (11 years)
Total awards	9	8	7	14	39	60
Awards with LDRD roots	5	6	4	9	23	36
% with LDRD roots	56%	75%	57%	64%	59%	60%
**Average years from first LDRD investment	6	5	3			

*Year to date: Each Laboratory has chosen the appropriate lookback period that will ensure data integrity.
**Los Alamos began tracking the years since first LDRD investment comprehensively in 2018.
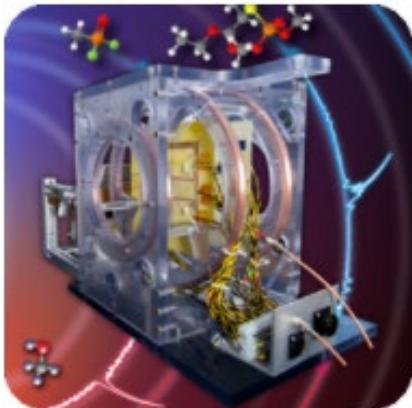
Why does this matter?
LDRD enables scientists and engineers to advance fundamental science with many possible applications. In this way, LDRD is the spark that sets many achievements in motion. Identifying the LDRD roots in R&D100 winners reflects the maturation of a concept from early R&D to an innovation with practical utility. The Laboratory technologies recognized by R&D 100 Awards often benefit many facets of society at-large.

In 2021, Los Alamos led seven R&D 100 winners, and four of the awards have roots in LDRD. These awards represent the program's investments in science, engineering, and technology impacting the broader scientific community. Below are the four 2021 winners with roots in LDRD.

Earth's-field Resonance Detection and Evaluation Device (ERDE)
Principal Investigators: Derrick Kaseman and Bob Williams

ERDE devices are portable nuclear magnetic resonance (NMR) spectrometers that use the Earth's magnetic field for rapid, accurate, and safe identification of chemicals without requiring superconducting magnets and liquid cryogens. Smaller than a microwave oven, ERDE devices have spectral resolutions equivalent to or higher than achieved with conventional superconducting NMR spectroscopy at a much lower cost, and can simultaneously collect signature data for all NMR-active nuclei in a single spectrum. These portable NMR spectrometers leverage heteronuclear J-couplings for applications in environmental sensing, through-pipe sensing, chemical analysis, toxic chemical detection, and compound structure identification. ERDE also received the Silver Special Recognition Award for Market Disruptor – Product, which highlights any product from any category that has changed the game in any industry.

The ERDE system was developed exclusively with LDRD support. The initial ERDE devices were developed under and LDRD Directed Research project (20170048DR) led by Robert Williams and titled, "Fieldable Chemical Threat Mapping by Multi-Modal Low Magnetic Field Nuclear Magnetic Resonance Signatures." The work continued under a LDRD Director's Postdoctoral Fellow Award to Derrick Kaseman (20190641PRD3) titled, "Development and Implementation of a Portable Microfluidic J-Coupled Spectrometer for Rapid Detection and Identification of Emerging Chemical Threats."

Video link: https://www.youtube.com/watch?v=vBmhtfM2PMM

Portable EnGineered Analytic Sensor with aUtomated Sampling (PEGASUS)
Principal Investigator: Harshini Mukundan

Conventional processing and analysis typically require well-equipped laboratories, trained personnel, and expensive equipment. The PEGASUS rugged, miniature biosensor detects a variety of important biomarkers, including bacterial signatures, viral genetic material, toxins, and potential biothreat agents. The simple-to-operate system uses a phone app for readout, analyzes a wide array of samples, and makes laboratory-quality analysis available anywhere. PEGASUS technology benefited from a LDRD project (20180387ER) led by Harshini Mukundan and titled, "Engineering the Universal Bacterial Sensor."

Video link: https://www.youtube.com/watch?v=SHfipRbOjbE

SmartTensors AI Platform
Principal Investigators: Boian Alexandrov and Velimir "Monty" Vesselinov

Crucial signals can be overlooked in big data. SmartTensors AI Platform uses unsupervised machine learning to transform and compress hundreds of trillions of data bytes into manageable pieces of information. Identifying hidden patterns in the data facilitates the discovery of new phenomena and new mechanisms, which enables informed decisions. Applications include analyses in medicine, disease spread and prediction, energy extraction, material science, carbon sequestration, climate change, economy, infrastructure stability, anomaly detection, text mining, and national security. SmartTensors AI Platform also won the Bronze Special Recognition Award for Market Disruptor – Services, which highlights any service from any category as one that forever changed the R&D industry or a particular vertical within the industry.

The SmartTensors software was developed under a LDRD project (20190020DR) led by Boian Alexandrov and titled, "Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics."

Video link: https://www.youtube.com/watch?v=ni3EgQVypbQ

Terra Spotlight
Principal Investigator: Amanda Ziemann

The software accomplishes what once seemed impossible: automatic identification of changes in satellite-based imagery collected from multiple independent imaging systems. The rigorous mathematical framework implicitly aligns the disparate sensing systems for multi-satellite, multi-physics data fusion and rapid discovery of important changes on the Earth's surface. Terra Spotlight uses more data collected from existing satellite imaging sensors, without requiring investment in additional expensive satellite platforms. Terra Spotlight also won also won the Silver Special Recognition Award for Market Disruptor – Services, which highlights any service from any category as one that forever changed the R&D industry or a particular vertical within the industry.

LDRD funded development of this technology through an Early Career Research project (20180529ECR) led by Amanda Ziemann and titled, "Geospatial Change Surveillance with Heterogeneous Data."

Video link: https://www.youtube.com/watch?v=EqZDUBG1bEI

Top 2%

A relevant indicator of career advancement in a ST&E field is the recognition of individuals as distinguished members of the technical staff. These staff members are named "Fellows" at LANL, Senior Scientists/Engineers at SNL, and Distinguished Members of the Technical Staff (DMTS) at LLNL. The shorthand name used here, "Top 2%," comes from the intent at each laboratory to limit membership to the top 1% or 2% of scientific and technical staff. Typically nominated and screened by a committee, the Top 2% are recognized for something similar to a lifetime achievement award, in this case, for contribution to the Laboratory's mission.

In FY21, three of the four LANL staff awarded the Fellow recognition had prior experience with LDRD. While there is sometimes minor fluctuation from year to year, multi-year analyses consistently reflect a high majority of Fellows with prior LDRD experience. At LANL, 47 of the 53 researchers who have been awarded APS fellowships since FY11 have prior experience with LDRD. Fellows typically gain LDRD experience early in their careers, with an average of about 13 years from their first LDRD experience to being named a Fellow.

History of Fellows at Los Alamos National Laboratory

	Single-Year Statistics			Multi-Year Statistics		
	FY19	**FY20**	**FY21**	**FY11-15 (5 years)**	**FY16-20 (5 years)**	**FY11-21* (11 years)**
Total awards	7	7	4	22	27	53
Awards with LDRD roots	6	7	3	19	25	47
% with LDRD roots	86%	100%	75%	86%	93%	89%
Average years from first LDRD experience	16.3	12.7	10.0	10.6	14.5	12.7

*Year to date: Each Laboratory has chosen the appropriate lookback period that will ensure data integrity.

Why does this matters?
Early involvement in LDRD has been found to have significant impact on career advancement, allowing participants unique opportunities to develop themselves and their ideas. Success in the national security enterprise depends on this world-class technical workforce.

Three of Four Researchers Elected as 2021 Fellows Have LDRD Experience

Four LANL scientists and engineers were elected as 2021 Laboratory Fellows. They represent top contributions made at the Laboratory.

Three of the elected Fellows have LDRD experience.

Baolian Cheng, of the Plasma Theory and Applications Group, has made sustained high-level contributions to national security and the Lab's mission over the past 25 years. Her discoveries have fundamentally affected the methodology for weapons certification. Throughout her career, Cheng has made vital contributions to hydrodynamic instabilities and mix, pit lifetime studies, primary certification metrics, primary boost metrics, and thermonuclear ignition metrics for inertial confinement fusion. Furthermore, she is a global expert on boost and ignition metrics, and is known for her strong foundational and first principles theoretical developments. Her work with LDRD began in 2008 when she was an investigator on a Directed Research project.

(First LDRD experience 2008)

Elizabeth Hunke, of the Lab's Fluid Dynamics and Solid Mechanics Group, is internationally recognized as the world's leading modeler of sea ice. Hunke leads the CICE Consortium, an international collaboration of sea ice modelers, and is a senior member the Lab's climate modeling team, which contributes cutting-edge research and development for the Department of Energy's Energy Exascale Earth System Model (E3SM) project. She has been a key force in mentoring two generations of climate team members. She also serves as the program manager for the Earth and Environmental Systems Sciences Division in DOE's Office of Science, a $30 million portfolio of experimental and modeling research. Her work with LDRD began in 2019 when she was an investigator on a Centers Research project.

(First LDRD experience 2019)

Blas Uberuaga, of the Materials Science in Radiation and Dynamics Extremes Group, has contributed for more than 20 years to the field of atomistic modeling of radiation effects in materials where he performed pioneering research in complex oxides and nanomaterials. He is the director of DOE's Fundamental Understanding of Transport Under Reactor Extremes (FUTURE), which researches the extreme conditions of irradiation and corrosion that impact materials in nuclear reactors. His scientific work to understand these effects continues to showcase the Laboratory's expertise. Additionally, he's shown exceptional leadership in the mentoring of 27 postdoctoral researchers and six graduate students. His work with LDRD began in 2007 when he was an investigator on an Exploratory Research project.

(First LDRD experience 2007)

Program Accomplishments

Top Science in the News

Despite the year's many challenges (and, in some cases, because of them), there were some incredible scientific and technological innovations out of Los Alamos in 2021. Here's a look back at just a few of the innovations supported by LDRD.

Mission to Mars!

An illustration of NASA's Perseverance rover landing safely on Mars. Los Alamos National Laboratory and LDRD have several critical roles on the mission. NASA/JPL-Caltech
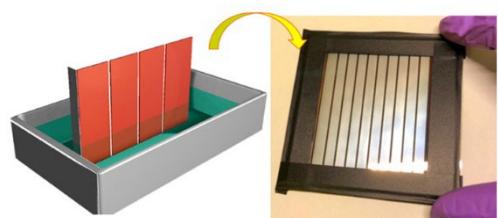
LDRD helps power Perseverance rover on Mars

While millions of people celebrated the [landing of the Perseverance rover on Mars](#), LDRD researchers at Los Alamos celebrated the 32 fuel pellets that will provide Perseverance safe and reliable power. Perseverance is one of many space instruments that depend on a Multi-Mission Radioisotope Thermoelectric Generator (MMRTG) — a type of nuclear battery that converts heat released by radioactive material into electricity. Each MMRTG requires 32 238PuO2 pellets that are produced at LANL. During the fabrication process, LANL has historically encountered a 15% pellet failure rate, which is largely a result of pellet cracking. An LDRD team led by Adam Parkison (20170531MFR) developed a customized computer model termed PUMA (Plutonium Modeling and Assessment), designed to simulate the full pellet fabrication process from ceramic powder through encapsulation. The PUMA simulation marks a distinct paradigm shift in how the 238PuO2 program approaches understanding the pellet production process.

Moving toward a clean-energy future

New fabrication method paves way to large-scale production of perovskite solar cells

A [new, simpler solution for fabricating stable perovskite solar cells](#) overcomes the key bottleneck to large-scale production and commercialization of this promising renewable-energy technology, which has remained tantalizingly out of reach for more than a decade. Work performed by Wanyi Nie and Shreetu Shrestha was supported by the LANL-LDRD program via project 20180026DR. "Our work paves the way for low-cost, high-throughput, commercial-scale production of large-scale solar modules in the near future," said LDRD researcher Wanyi Nie, who is the corresponding author of the paper, which was recently published in the journal [Joule](#).

A new dipping process using a sulfolane additive creates high-performing perovskite solar cells. The method is inexpensive and well-suited for scaling up to commercial production.

Using climate science to assess our changing world
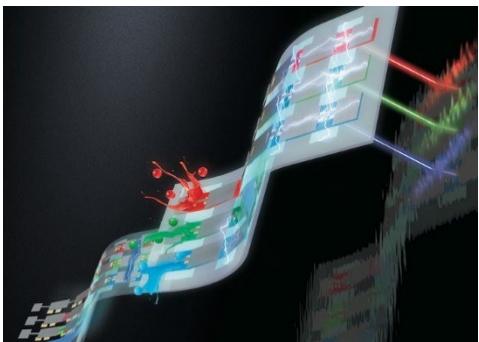
Colorado River basin due for more frequent, intense hydroclimate events

[Changes in climate extremes and climate disturbances can cause catastrophic damage](#) to social and ecological systems and are becoming increasingly common and intense at global and regional scales. LDRD researcher Katrina Bennett works to estimate changing extremes, using multiple statistical techniques, and projects extremes are expected to increase dramatically for the Colorado River basin, a critical watershed to the US economy. Adaptation measures can help planners and managers better prepare for changing extremes, reducing costs associated with damages.
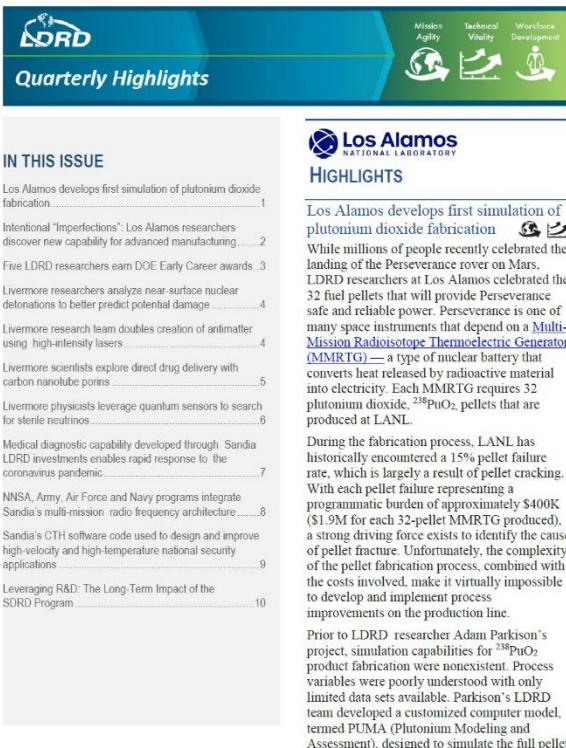
Coming of age, technologies on the horizon

Colloidal quantum dot lasers poised to come of age

A new paper by authors from Los Alamos and Argonne national laboratories sums up the [recent progress in colloidal-quantum-dot research](#) and highlights the remaining challenges and opportunities in the rapidly developing field, which is poised to enable a wide array of new laser-based and LED-based technology applications. "Colloidal quantum dot lasers have tremendous potential in a range of applications, including integrated optical circuits, wearable technologies, lab-on-a-chip devices, and advanced medical imaging and diagnostics," said Victor Klimov, LDRD researcher and lead author of the [cover article](#) in *Nature Photonics*.

Research Highlights

Stay apprised of the latest technical advances, mission-impact success stories, and notable staff achievements of the NNSA's premier internal investment resource for high-risk, potentially high-payoff research and development.

The LDRD Quarterly Highlights newsletter is intended to inform decision makers, foster technology adoption by national security and defense program managers, and enable all readers to:

- Track the development of new and expanding capabilities.
- See how others have implemented recent advances.
- Learn about the programs, products, and collaborations inspired by our leading-edge R&D.

Each story identifies the objectives it best illustrates: mission agility, Technical vitality, workforce development.

FY21 Project Summaries

For FY21 project summaries see the stand-alone compendium available at:
https://www.lanl.gov/projects/ldrd-tri-lab/annual-reports.php.

End Overview Section

FY21 Project Summaries

Complex Natural and Engineered Systems

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

Gian Delzanno
20200073DR

Project Description

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

Publications

Journal Articles

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

Borovsky, J. E., G. L. Delzanno and K. Yakymenko. Pitch-Angle Diffusion in the Earth's Magnetosphere Organized by the Mozer-Transformed Coordinate System. Submitted to *Frontiers Astronomy and Space Sciences*. (LA-UR-21-31107)

Broll, J. M. and G. S. Cunningham. Inner belt electron decay timescales: a comparison of Van Allen Probes and DREAM3D losses following the June 2015 storm. Submitted to *Geophysical Research Letters*. (LA-UR-22-22470)

Colestock, P., G. L. Delzanno, Q. R. Marksteiner, K. A. Shipman and N. Yampolsky. A Comparison of Wave Emitters for Applications in the Inner Magnetosphere. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-21-20126)

Colestock, P., G. L. Delzanno and N. Yampolsky. On the Calculation of Antenna Impedance for Applications in the Inner Magnetosphere. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-21-20129)

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

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

Cunningham, G. S., E. Botek, V. Pierrard, C. M. Cully and J. Ripoll. Observation of High-Energy Electrons Precipitated by NWC Transmitter from PROBA-V Low-Earth Orbit Satellite. Submitted to *Geophysical Research Letters*. (LA-UR-20-23776)

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

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

*Pierrard, V., E. Botek, J. -. Ripoll and G. Cunningham. Electron Dropout Events and Flux Enhancements Associated With Geomagnetic Storms Observed by PROBA-V/Energetic Particle Telescope From 2013 to 2019. 2020. *Journal of Geophysical Research: Space Physics*. **125** (12). (LA-UR-20-24439 DOI: 10.1029/2020JA028487)

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

D. Reeves, E. G. Earth's Radiation Belts: The Hazards to Satellites and What Can Be Done to Mitigate the Risks?.

Submitted to *Proceedings of the AMOS conference*. (LA-UR-20-26784)

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

*Reeves, G. D., E. M. Vandegriff, J. T. Niehof, S. K. Morley, G. S. Cunningham, M. G. Henderson and B. A. Larsen. Defining Radiation Belt Enhancement Events Based on Probability Distributions. 2020. *Space Weather*. **18** (8): e2020SW002528. (LA-UR-20-24379 DOI: 10.1029/2020SW002528)

*D. G. L. Roytershteyn, V. *. and G. L. Delzanno. Nonlinear coupling of whistler waves to oblique electrostatic turbulence enabled by cold plasma. 2021. *Physics of Plasmas*. **28** (4): 42903. (LA-UR-20-20992 DOI: 10.1063/5.0041838)

Reports

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

Presentation Slides

Broll, J. M., G. S. Cunningham, D. Malaspina, E. G. D. Reeves, M. G. Henderson and G. L. Delzanno. Validating DREAM3D simulations of inner belt dynamics. Presented at *American Geophysical Union Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31867)

Broll, J. M. and B. Walsh. Refining predictions of reconnection X-lines at Earth's magnetopause. Presented at *MMS SWT 2020*, San Antonio, Texas, United States, 2020-10-06 - 2020-10-08. (LA-UR-20-27886)

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

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

Cunningham, G. S., C. A. M. Jeffery and L. Y. Khoo. Predicting the effect of the NWC transmitter on relativistic electrons using DREAM3D. Presented at *2021 Fall Meeting of the American Geophysical Union*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31991)

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

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

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

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

Delzanno, G. L. Overview of RBR-ACES. . (LA-UR-21-20199)

Delzanno, G. L. Advanced modeling in support of space missions - part 2 -. . (LA-UR-21-25614)

Delzanno, G. L. Preliminary comparison of wave power with LAPD experiments. . (LA-UR-21-28334)

Delzanno, G. L. Radiation Belt Remediation Using Artificially Generated Plasma Waves. Presented at *AGU fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31922)

Delzanno, G. L., J. E. Borovsky, G. Miars and B. Gilchrist. Active experiments in space with relativistic electron accelerators. Presented at *AAPPS-DPP2021*, Online, Japan, 2021-09-27 - 2021-09-27. (LA-UR-21-29571)

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

Delzanno, G. L., Q. R. Marksteiner, E. G. D. Reeves, J. M. Broll, P. L. Colestock, M. Cowee, G. S. Cunningham, L. D. Duffy, X. Fu, J. C. Holmes, C. A. M. Jeffery, O. Koshkarov, K. A. Shipman, D. Svyatsky, H. Xu, K. Yakymenko, N. Yampolsky, S. Dorfman, G. Ginet and V. Roytershteyn. Radiation Belt Remediation Using Artificially Generated Plasma Waves. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31866)

Delzanno, G. L., Q. R. Marksteiner, E. G. D. Reeves, J. M. Broll, P. L. Colestock, M. Cowee, G. S. Cunningham, L. D. Duffy, X. Fu, J. C. Holmes, C. A. M. Jeffery, O. Koshkarov, K. A. Shipman, D. Svyatsky, H. Xu, K. Yakymenko, N. Yampolsky, S. Dorfman, G. Ginet and V. Roytershteyn. Radiation Belt Remediation Using Artificially Generated Plasma Waves. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31872)

Delzanno, G. L., Q. R. Marksteiner, G. D. Reeves, B. E. Carlsten, P. L. Colestock, M. Cowee, G. S. Cunningham, L. D. Duffy, C. A. M. Jeffery, O. Koshkarov, K. A. Shipman, D. Svyatsky, K. Yakymenko, N. Yampolsky, J. M. Albert, C. Crabtree, S. Dorfman, J. McCollough and V. Roytershteyn. Recent progress towards a radiation belt remediation strategy based on artificial injection of plasma waves. Presented at *American Geophysical Union Fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-32261)

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

Delzanno, G. L., V. Roytershteyn and K. Yakymenko. Electron-beam/plasma coupling physics in support of active

experiments in space. Presented at *ICEAA*, honolulu, Hawaii, United States, 2021-08-09 - 2021-08-09. (LA-UR-21-26703)

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

Delzanno, G. L. and V. Roytershteyn. The impact of cold electrons on whistler waves. Presented at *URSI-GASS*, Rome, Italy, 2021-08-28 - 2021-08-28. (LA-UR-21-28169)

Delzanno, G. L. and V. Roytershteyn. The impact of cold electrons on whistler waves. Presented at *URSI-GASS*, Rome, Italy, 2021-08-28 - 2021-08-28. (LA-UR-21-28170)

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

Fu, X., G. S. Cunningham, M. Cowee, E. G. D. Reeves and G. L. Delzanno. Interactions of Artificially-Generated Whistler Waves with Radiation Belt Electrons. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32227)

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

Holmes, J. C., G. L. Delzanno, C. A. M. Jeffery and P. L. Colestock. Using Ray Tracing to Model the Plasmaspheric Wave Field for Active Experiments in Space. Presented at *ICEAA IEEE APWC USNC URSI RSM 2021 VIRTUAL*, Honolulu, Hawaii, United States, 2021-08-09 - 2021-08-31. (LA-UR-21-26411)

Holmes, J. C., G. L. Delzanno, C. A. M. Jeffery and P. L. Colestock. Using Ray Tracing to Model the Plasmaspheric Wave Field for Active Experiments in Space. Presented at *ICEAA IEEE APWC USNC URSI RSM 2021 VIRTUAL*, Honolulu, Hawaii, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-26777)

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

Marksteiner, Q. R., B. E. Carlsten, P. L. Colestock, G. L. Delzanno, S. Dorfman, L. D. Duffy, M. A. Holloway, J. W. I. Lewellen, D. Nguyen, E. G. D. Reeves, V. Roytershteyn, N. Yampolsky and H. Xu. Space-Borne Accelerators. Presented at *UK Accelerator Institutes Seminar*, Online, New Mexico, United States, 2022-03-03 - 2022-03-03. (LA-UR-22-21894)

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

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

D. Reeves, E. G. Wave Generation and Wave-Particle Interaction Using Space-Based, \xe2\x80\xa8RF, Linear Electron Accelerators. Presented at *The twenty-second edition of the International Conference on Electromagnetics in Advanced Applications (ICEAA 2021)*, Honolulu, Hawaii, United States, 2021-08-08 - 2021-08-08. (LA-UR-21-28486)

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

Roytershteyn, V. and G. L. Delzanno. Nonlinear Coupling of Whistler Waves to Oblique Electrostatic Turbulence Enabled by Cold Plasma. Presented at *International Conference on Electromagnetics in Advanced Applications (ICEAA)*, honolulu, Hawaii, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-26391)

Roytershteyn, V. and G. L. Delzanno. Nonlinear Coupling of Whistler Waves to Oblique Electrostatic Turbulence Enabled by Cold Plasma. Presented at *ICEAA 2021*, honolulu, Hawaii, United States, 2021-08-09 - 2021-08-09. (LA-UR-21-26464)

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

Posters

Delzanno, G. L. and V. Roytershteyn. The impact of cold electrons on whistler waves. Presented at *American Geophysical Union Fall meeting*, New Orleans, Louisiana, United States, 2021-12-12 - 2021-12-12. (LA-UR-21-31628)

Holmes, J. C., G. L. Delzanno, P. L. Colestock, G. P. Ginet, M. J. Starks and W. R. Johnston. Constraints on the DSX Antenna Pattern Using Boomerang E-field Measurements and Linear Theory. Presented at *American Geophysical Union Fall Meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31417)

Holmes, J. C., G. L. Delzanno and P. L. Colestock. How do we handle magnetospherically reflected waves in ray-tracing models?. Presented at *GEM Virtual Conference 2021*, Santa Fe, New Mexico, United States, 2021-07-26 - 2021-07-30. (LA-UR-21-27258)

Shipman, K. A., P. Colestock, N. Yampolsky, L. D. Duffy, M. A. Gilmore, Q. R. Marksteiner and G. L. Delzanno. Curvilinear Particle-in-Cell Simulations of Plasma Sheath Effects on Impedance of VLF Antenna in Magnetosphere. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32099)

Yampolsky, N., P. L. Colestock, Q. R. Marksteiner, K. A. Shipman and G. L. Delzanno. Excitation of whistler waves in Earth magnetosphere with antennas. Presented at *APS meeting, Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-07 - 2021-11-12. (LA-UR-21-31037)

Directed Plant-Microbiome Evolution for Food and Biofuel Security

Sanna Sevanto
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Project Description

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

Publications

Journal Articles

Carter, K. R. and L. T. Dickman. Recovery of seedling carbon balance despite hydraulic impairment following hot drought. Submitted to *Tree Physiology*. (LA-UR-21-32295)

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

Kim, A., E. R. Moore, S. A. Sevanto and N. E. Lubbers. Topic modeling of soil microbiomes in droughted corn.
Submitted to *Computational and Structural Biotechnology Journal*. (LA-UR-21-31781)

Nakad, M., J. C. Domec, S. A. Sevanto and G. Katul. A radial-axial transport coordination enhances sugar translocation in the phloem vasculature of plants. Submitted to *Plant Physiology*. (LA-UR-21-28873)

*Nakad, M., T. Witelski, J. C. Domec, S. Sevanto and G. Katul. Taylor dispersion in osmotically driven laminar flows in phloem. 2021. *Journal of Fluid Mechanics*. **913**: A44. (LA-UR-20-23039 DOI: 10.1017/jfm.2021.56)

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

Sevanto, S. A. Flow resistance of phloem sieve plates revisited. Submitted to *Journal of Plant Physiology*. (LA-UR-22-20429)

Sevanto, S. A., C. Gehring, M. G. Ryan, A. Patterson, A. Losko, S. C. Vogel, K. R. Carter, L. T. Dickman, M. A. Espy and C. R. Kuske. Ectomycorrhizal root colonization differentially affects water uptake and drought tolerance in drought tolerant and intolerant pinyon pine genotypes. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-21-31041)

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

Ulrich, D., C. Clandinen, F. Algoni, R. Mueller, R. Chu, J. Toyoda, L. A. Gallegos-Graves, H. Goemann, B. Peyton, S. A. Sevanto and J. M. Dunbar. Root exudate composition reflects drought severity gradient in blue grama (Bouteloua gracilis). Submitted to *New Phytologist*. (LA-UR-21-31831)

Conference Papers

Kim, A., S. A. Sevanto and N. E. Lubbers. Topic modeling of soil microbiomes in droughted corn. Presented at *AAAI 2021 Fall Symposium*. (Arlington, Virginia, United States, 2021-11-04 - 2021-11-06). (LA-UR-21-28491)

Kim, A., S. A. Sevanto and N. E. Lubbers. Topic modeling of soil microbiomes in droughted corn. Presented at *AAAI*

2021 Fall Symposium. (Arlington, Virginia, United States, 2021-11-04 - 2021-11-06). (LA-UR-21-28491)

Presentation Slides

Carter, K. R., L. Comas, J. P. Heneghan, L. T. Dickman, E. R. Moore, A. C. Nachtsheim, D. Musa, A. J. Sabella, M. B. N. Albright, C. R. Steadman, J. M. Heikoop, B. D. Newman, S. N. Twary, N. E. Lubbers, S. Negi, C. M. Yeager, J. M. Dunbar and S. A. Sevanto. Microbiome effects on maize form and function under altered watering conditions. Presented at *Ecological Society of American Annual Meeting*, Long Beach, California, United States, 2021-08-02 - 2021-08-06. (LA-UR-21-26675)

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

Mitchell, J. M. Filling our Knowledge Gaps in Metabolism to Secure Food and Biofuel Security. . (LA-UR-21-28066)

Mitchell, J. M. Leveraging 2-D GC-MS and Machine Learning to Explore the Corn Metabolome. . (LA-UR-22-21078)

Nakad, M., J. C. Domec, S. A. Sevanto and G. Katul. A concentration dependent viscosity enhances the resilience of phloem hydraulic to sucrose loading. Presented at *Annual meeting of the Ecological Society of America*, Los Alamos, New Mexico, United States, 2021-08-02 - 2021-08-02. (LA-UR-21-26468)

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

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

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

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

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

Posters

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

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

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

Other

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

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

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Project Description

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

Publications

Journal Articles

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

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

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

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

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

Qiao, Z., C. Li, C. Wang, S. Hwang, B. Li, Y. Zeng, A. J. Kropf, C. E. Wegener, Q. Gong, G. Wang, D. Myers, J. Xie, J. S. Spendelow and G. Wu. Synergistic PGM-free Single Metal Sites for Promoting PtCo Ordered Intermetallic Fuel Cell Catalysts: Performance and Durability Improvements. Submitted to *Energy & Environmental Science*. (LA-UR-21-23020)

Qiao, Z., C. Wang, Y. Zeng, J. S. Spendelow and G. Wu. Advanced Nanocarbons for Enhanced Performance and Durability of Platinum Catalysts in Proton Exchange Membrane Fuel Cells. 2021. *Small*. 2006805. (LA-UR-21-22987 DOI: 10.1002/smll.202006805)

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

Presentation Slides

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

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

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

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

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

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

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

Model-Driven Data Fusion for Disease Forecasting

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Project Description

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

Publications

Journal Articles

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

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

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

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

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

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

Hepler, S., K. A. Kaufeld, K. Benedict, M. Toda, B. R. Jackson, X. Liu and D. Kline. INTEGRATING PUBLIC HEALTH SURVEILLANCE AND ENVIRONMENTAL DATA TO MODEL PRESENCE OF HISTOPLASMA IN THE UNITED STATES. Submitted to *Epidemiology*. (LA-UR-21-26964)

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

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

Temple, S. D. and K. A. Kaufeld. Bayesian time-varying occupancy model for West Nile virus in Ontario, Canada. Submitted to *Stochastic Environmental Research and Risk Assessment*. (LA-UR-21-31764)

Conference Papers

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

Reports

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

Presentation Slides

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

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

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

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

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

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

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

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

Martinez, K. M., C. A. Manore, S. Y. Del Valle, G. Fairchild, A. Ziemann, N. K. Parikh, L. A. Castro, K. C. Kempfert, D.

A. Romero-Alvarez and E. N. A. Generous. Data Fusion and Disease Forecasting for Dengue in Brazil. . (LA-UR-21-31403)

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

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

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

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

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

Posters

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

Other

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

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

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

Shawn Starkenburg
20210082DR

Project Description

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

Publications

Journal Articles

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

Micheva-Viteva, S. N., A. S. Bell and S. R. Starkenburg. Nonclassical autophagy activation pathways are essential for production of infectious Influenza A virus in vitro. 2021. *Molecular Microbiology*. (LA-UR-20-30117 DOI: 10.1111/mmi.14865)

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

Reports

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

Presentation Slides

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

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

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

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

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

Posters

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

Advanced Characterization to Enable Prediction of Actinide-Molten Salt Behavior

Marisa Monreal
20210113DR

Project Description

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

Publications

Journal Articles

R. Andersson, A. D. and B. Beeler. Ab initio molecular dynamics (AIMD) simulations of NaCl, UCl3 and NaCl-UCl3 molten salts. Submitted to *Journal of Nuclear Materials*. (LA-UR-22-20387)

J. Lhermitte, C. R., S. S. Parker, J. M. Jackson and M. J. Monreal. Mg+2/0 as a reliable reference electrode for chloride melts. Submitted to *Journal of the Electrochemical Society*. (LA-UR-21-20290)

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

Vogel, S. C., A. D. R. Andersson, M. J. Monreal, J. M. Jackson, S. S. Parker, G. Wang, P. Yang and J. Zhang. Crystal Structure Evolution of UCl3 from Room Temperature to Melting. Submitted to *JOM*. (LA-UR-21-24639)

Vogel, S. C., M. J. Monreal and A. P. Shivprasad. Materials for Small Nuclear Reactors and Micro Reactors, including Space Reactors. Submitted to *JOM*. (LA-UR-21-28723)

Conference Papers

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

Presentation Slides

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

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

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

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

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

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

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

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

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

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

Posters

Yankey, J., M. J. Monreal, J. M. Jackson, S. S. Parker, S. Choi and M. Simpson. Measurement of Vapor Pressure of UCl3 in NaCl-MgCl2-UCl3 via Transpiration Experiments. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-21475)

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

Hongwu Xu
20180007DR

Project Description

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

Technical Outcomes

This project has opened a new field in high Pressure-Temperature (P-T) aqueous actinide research. We pioneered unprecedented, in-situ measurements and multiscale modeling of actinide solubility, speciation and stability under P-T regimes relevant to a range of issues in actinide applications. The results have uncovered properties that are completely different from those predicted by extrapolation of existing room P-T behavior, and thus have reimaged conventional wisdom of actinide behavior in water-mediated processes at high P-T conditions.

Publications

Journal Articles

*Instability of U3Si2 in pressurized water media at elevated temperatures. 2021. *Communications Chemistry*. **4** (1): 65. (LA-UR-20-27557 DOI: 10.1038/s42004-021-00504-3)

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

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

Baker, J. L., J. T. White, A. Chen, T. Ulrich, R. R. Roback and H. Xu. Heat capacity, entropy, formation energy and spin-fluctuation behavior of U3Si5 from 2.4 to 397.4 K. 2021. *Journal of Nuclear Materials*. **557**: 153282. (LA-UR-21-24852 DOI: 10.1016/j.jnucmat.2021.153282)

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

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

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

*Dhakal, D., R. A. Mayanovic, J. L. Baker, H. Boukhalfa, H. Xu and C. Sun. Design of a containment apparatus for synchrotron XAS measurements of radioactive fluid samples under high temperatures and pressures. 2019.

Review of Scientific Instruments. **90** (8): 083108. (LA-UR-19-23291 DOI: 10.1063/1.5100887)

*. S. A. *. D. J. *. P. A. *. X. H. *. M. A. Gabitov, R. I., H. Xu and A. Migdisov. Sectoral and growth rate control on elemental uptake by individual calcite crystals. 2021. *Chemical Geology*. **585**: 120589. (LA-UR-21-28232 DOI: 10.1016/j.chemgeo.2021.120589)

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

. W. N. *. L. M. L. *. E. S. M. *. M. A. *. X. H. *. L. M. *. G. X. Goncharov, V. G., H. Xu, V. G. Goncharov and A. Migliori. Elastic and thermodynamic properties of cerium-doped yttrium aluminum garnets. 2021. *Journal of the American Ceramic Society*. **104 (7): 3478-3496. (LA-UR-20-24352 DOI: 10.1111/jace.17679)

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

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

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

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

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

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

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

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

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

*Migdisov, A. A., W. Runde, A. E. Williams-Jones, H. Boukhalfa, R. Roback and A. Timofeev. Response to the comment "Uranyl-chloride speciation and uranium transport in hydrothermal brines: Comment on Migdisov et al. (2018)" by Dargent et al.. 2018. *Geochimica et Cosmochimica Acta*. **235**: 509-512. (LA-UR-18-21513 DOI: 10.1016/j.gca.2018.06.015)

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

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

Nisbet, H. D., A. Migdissov, A. E. Williams-Jones, V. van Hinsberg, H. Xu and R. C. Roback. The solubility of thorium in carbonate-bearing solutions at hydrothermal conditions. 2021. *Geochimica et Cosmochimica Acta*. (LA-UR-20-30269 DOI: 10.1016/j.gca.2021.04.035)

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

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

SUBRAMANI, T., J. L. Baker, H. Xu and A. Navrotsky. Synthesis, characterization, and enthalpies of formation of uranium substituted zirconolites. Submitted to *ACS Earth and Space Chemistry*. (LA-UR-20-24973)

Strzelecki, A. C., T. Barral, A. Mesbah, V. Goncharov, J. L. Baker, J. Bai, P. Estevenon, S. Szenknect, A. Migdissov, H. Xu, R. C. Ewing, N. Dacheux and X. Guo. Role of water and hydroxyl groups in the structures of stetindite and coffinite, MiSiO4 (M = Ce, U). Submitted to *Chemistry of Materials*. (LA-UR-20-27006)

*Timofeev, A., A. A. Migdisov, A. E. Williams-Jones, R. Roback, A. T. Nelson and H. Xu. Uranium transport in acidic brines under reducing conditions. 2018. *Nature Communications*. **9** (1): 1469. (LA-UR-17-29029 DOI: 10.1038/s41467-018-03564-7)

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

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

*Xiaofeng, G., H. Boukhalfa, J. N. Mitchell, M. Ramos, A. J. Gaunt, A. Migliori, R. C. Roback, A. Navrotsky and X. Hongwu. Sample seal-and-drop device and methodology for high temperature oxide melt solution calorimetric measurements of PuO. 2019. *Review of Scientific Instruments*. **90** (4): 44101. (LA-UR-19-21351 DOI: 10.1063/1.5093567)

Xu, H. Trisulfur radical anion S3\xe2\x80\xa2− -- A major carrier for platinum in hydrothermal fluids. Submitted to *PNAS*. (LA-UR-21-27326)

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

*Xu, H., X. L\xc3\xbc, P. J. Heaney and Y. Ren. Structural behavior of a stuffed derivative of \xce\xb1-quartz, Mg0.5AlSiO4, at high temperature: an in situ synchrotron XRD study. 2019. *Physics and Chemistry of Minerals*. **46** (7): 717-725. (LA-UR-19-21198 DOI: 10.1007/s00269-019-01033-1)

Books/Chapters

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

Presentation Slides

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Migdissov, A., X. Guo, H. D. Nisbet, N. F. van Hartesveldt, A. Kalintsev, H. Xu, H. Boukhalfa, R. C. Roback, V. van Hinsberg, A. E. Williams-Jones, R. I. Gabitov and J. Brugger. Geochemical controls of mobilisation, deposition, and fractionation of REE, U, and Th in ore forming hydrothermal systems. Presented at *Goldschmidt 2018*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-18. (LA-UR-18-27542)

Nisbet, H. D., A. Migdissov, A. E. Williams-Jones, V. van Hinsberg and H. Xu. The Solubility of Thorium in Carbonate-Bearing Solutions at Hydrothermal Conditions. Presented at *Goldschmidt Conference (Virtual)*, Los Alamos, New Mexico, United States, 2021-07-04 - 2021-07-09. (LA-UR-21-25841)

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

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

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

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

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

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

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

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

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

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

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

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

Xu, H., X. Guo, C. Chung, J. T. White, J. N. Mitchell, H. Boukhalfa, A. J. Gaunt, A. Migdissov, G. Wang, P. Yang, E. R. Batista and A. Navrotsky. Calorimetric Studies of Actinide Compounds.

Presented at *LDRD DR Project Appraisal Meeting*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20543)

Posters

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

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

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

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

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

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

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

Other

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

Adaptation Science for Complex Natural-Engineered Systems

Donatella Pasqualini
20180033DR

Project Description

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

Technical Outcomes

The project developed a transformative coastal adaptation framework for addressing climate impacts on coastal energy and water infrastructure. The project achieved this goal by developing new capabilities to model a dynamic coastal landscape that integrates vegetation, ocean, and land; and a new capability for designing resilient regional infrastructures based on infrastructure network optimization and physics-based uncertainty quantification of natural hazards. The new integrated framework enables the limitations of current adaptation planning approaches to be overcome.

Publications

Journal Articles

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

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

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

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

*Francom, D. and B. Sanso. BASS: An R Package for Fitting and Performing Sensitivity Analysis of Bayesian Adaptive Spline Surfaces. 2020. *Journal of Statistical Software*. **94** (8). (LA-UR-20-23587 DOI: 10.18637/jss.v094.i08)

*Hanson, P. C., A. B. Stillman, X. Jia, A. Karpatne, H. A. Dugan, C. C. Carey, J. Stachelek, N. K. Ward, Y. Zhang, J. S. Read and V. Kumar. Predicting lake surface water phosphorus dynamics using process-guided machine learning. 2020. *Ecological Modelling*. **430**: 109136. (LA-UR-20-25013 DOI: 10.1016/j.ecolmodel.2020.109136)

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

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

Tasseff, B. A., R. W. Bent, M. A. Epelman, D. Pasqualini and P. Van Hentenryck. Exact Mixed-integer Convex Programming Formulation for Optimal Water Network Design (Companion). Submitted to *INFORMS Journal on Optimization*. (LA-UR-20-27433)

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

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

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

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

*Zhang, Y., J. C. Rowland, C. Xu, P. J. J. Wolfram, D. Svyatsky, J. D. Moulton, M. Marani, A. D'Alpaos, Z. Cao and D. Pasqualini. Understanding the eco-geomorphologic feedback of coastal marsh under sea level rise: vegetation dynamic representations, processes interaction, and parametric sensitivity. 2020. *Journal of Geophysical Research: Earth Surface*. e2020JF005729. (LA-UR-19-28502 DOI: 10.1029/2020JF005729)

Reports

Tasseff, B. A., R. W. Bent, M. A. Epelman, D. Pasqualini and P. Van Hentenryck. Exact Mixed-integer Convex Programming Formulation for Optimal Water Network Design. Unpublished report. (LA-UR-20-27823)

Tasseff, B., R. Bent, D. Pasqualini, M. A. Epelman and P. Van Hentenryck. Exact Mixed-integer Convex Programming Formulation for Optimal Water Network Design. Unpublished report. (LA-UR-20-24284)

Presentation Slides

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

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

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

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

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

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

Tasseff, B. A. Optimization of Critical Infrastructure with Fluids. . (LA-UR-21-26827)

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

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

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

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

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

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

Urban, N. M., D. Pasqualini and J. C. Rowland. Coastal infrastructure adaptation: High-fidelity endogenous modeling of coastal energy-water infrastructure adaptation. Presented at *National Renewable Energy Laboratory LDRD collaborative meeting*, Golden, Colorado, United States, 2018-10-04 - 2018-10-04. (LA-UR-18-30331)

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

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

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

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

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

J. Wolfram, P. J., S. R. Brus, G. Bisht, Z. Tan and T. Zhou. E3SM Coastal Waves mini-NGD:Toward simulation of regional sea level rise and inundation through coupled wave modeling and Science in Earth System Model Development (ESMD). Presented at *NOAA Collaboration Discussion (on web)*, Los Alamos, New Mexico, United States, 2020-05-21 - 2020-05-21. (LA-UR-20-23804)

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

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

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

J. Wolfram, P. J., T. Zhou, G. Bisht, Z. Cao, Z. Tan, H. Li, C. Liao, L. Zhai, A. F. Roberts, J. D. Wolfe, M. R. Petersen, B. Arbic, D. Engwirda, S. R. Brus, M. E. Maltrud, X. S. Asay-Davis, R. Leung and I. Kraucunas. Global to coastal multiscale modeling in the Energy Exascale Earth System Model. Presented at *E3SM Nov Project Meeting*, Washington, District Of Columbia, United States, 2019-11-19 - 2019-11-21. (LA-UR-19-31392)

Xu, C. Improved representation of vegetation dynamics in Earth System Models. Presented at *Invited department seminar at Department of Civil and Environmental Engineering*, Houston, Texas, United States, 2019-04-05 - 2019-04-05. (LA-UR-19-23209)

Xu, C., L. Zhai, J. C. Rowland and D. Pasqualini. Assessing the vulnerability of coastal vegetation climate change using a dynamic vegetation model. Presented at *2019 AGU*, San Francisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-32408)

Posters

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

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

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

J. Wolfram, P. J., S. R. Brus, Z. Cao, M. R. Petersen, M. E. Maltrud, L. Van Roekel, J. C. Rowland, D. Pasqualini, N. M. Urban, Z. Yang, J. D. Moulton, D. Svyatsky, C. Xu, R. W. Bent, B. Li, B. A. Tasseff and D. C. Francom. Coastal modeling through novel ocean developments in E3SM. Presented at *DOE EESM PI meeting*, Potomac, Maryland, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30478)

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

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

Other

Moulton, J. D., E. Coon, S. L. Painter, R. V. Garimella, S. Molins, K. Lipnikov, D. Svyatsky, V. Freedman, D. R. Harp, A. L. Atchley and Z. Lu. Summary for Amanzi-ATS R&D 100 Video Entry. Audio/Visual. (LA-UR-20-25076)

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

BioManufacturing with Intelligent Adaptive Control: BioManIAC

Babetta Marrone
20190001DR

Project Description

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

Technical Outcomes

The main goal was achieved, to develop machine learning (ML) models and simulations that enabled insight into the chemical structure-property relationships of an emerging class of biopolymers, the polyhydroxyalkanoates (PHAs), and the genes regulating their biosynthesis. New knowledge of PHA degradation by environmental conditions, both through experiments and ML models, was gained. The advancements made in understanding the PHA class of biopolymers will provide new insights into future biopolymer design that balances performance with degradation.

Publications

Journal Articles

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

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

Gonzalez Esquer, C. R., B. Ferlez, S. Weraduwage, H. Kirst, A. T. Lantz, A. Turmo, T. D. Sharkey and C. A. Kerfeld. Validation of an insertion-engineered isoprene synthase as a strategy to functionalize terpene synthases. 2021. *RSC Advances*. **11** (48): 29997-30005. (LA-UR-20-22812 DOI: 10.1039/D1RA05710C)

Hernandez, M. M., N. S. Gupta, K. Lee, A. C. Pital, B. L. Marrone, C. N. Iverson and J. H. Dumont. Characterization of Polyhydroxybutyrate-based Composites Prepared by Injection Molding. Submitted to *Polymers*. (LA-UR-21-28581)

Kuenneth, C., J. N. Lalonde, B. L. Marrone, C. N. Iverson, R. Ramprasad and G. Pilania. Bioplastic Design using Multitask Deep Neural Networks. Submitted to *Communications Materials*. (LA-UR-22-21336)

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

Marrone, B. L. The Year of Listening Differently. Submitted to *Science*. (LA-UR-21-24235)

Marrone, B. L., Z. Jiang, G. Pilania, J. Hu and X. (. Yu. A Deep Neural Network for Accurate and Robust Prediction of the Glass Transition Temperature of Polyhydroxyalkanoate Homo- and Co-Polymers. Submitted to *Omega ACS*. (LA-UR-20-25907)

Pilania, G. Machine Learning in Materials Science: From Explainable Predictions to Autonomous Design. Submitted to *Computational Materials Science*. (LA-UR-20-28959)

*Pilania, G., B. L. Marrone and C. N. Iverson. Machine-Learning-Based Predictive Modeling of Glass Transition Temperatures: A Case of Polyhydroxyalkanoate Homopolymers and Copolymers. 2019. *Journal of Chemical Information and Modeling*. **59** (12): 5013-5025. (LA-UR-19-28291 DOI: 10.1021/acs.jcim.9b00807)

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

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

Books/Chapters

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

Presentation Slides

Sudasinghe Appuhamilage, N. M., C. R. Gonzalez Esquer, L. L. Jacobs, S. Banerjee, T. M. Yoshida, G. Pilania, J. P. Theiler, R. K. Jha, S. R. Starkenburg, T. T. Dale and B. L. Marrone. Evaluation of the Role of Non-Intuitive Genes in Cyanobacterial Polyhydroxybutyrate Biosynthesis. Presented at *International Conference on Algal Biomass, Biofuels and Bioproducts (AlgalBBB 2021)*, Online, New Mexico, United States, 2021-06-14 - 2021-06-16. (LA-UR-21-25530)

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

Banerjee, S. Protein engineering for public health and energy security. . (LA-UR-21-24996)

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

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

Dale, T. T. High Throughput Screening Applications in Biomanufacturing. Presented at *CNES Capability Deep Dive*, Los Alamos, NM, New Mexico, United States, 2021-05-07 - 2021-05-07. (LA-UR-21-23574)

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

Dumont, J. H. Introducing Bioplastics at LANL. . (LA-UR-21-27283)

Dumont, J. H. Discovering New Biodegradable Plastics. . (LA-UR-21-27562)

Gonzalez Esquer, C. R. Reconfiguring the metabolism of photosynthetic microbes for their development as biotechnological platforms. . (LA-UR-21-28107)

Hernandez, M. M., N. S. Gupta, K. Lee, B. L. Marrone, C. N. Iverson and J. H. Dumont. Engineering a Greener Future: Biodegradable Polyhydroxybutyrate Composites. Presented at *LANL Student Symposium 2021*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27527)

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

Kuenneth, C. B., G. Pilania, C. N. Iverson, B. L. Marrone and R. Ramprasad. Polymer Informatics with Multitask Deep Neural Networks to Design Bioplastics. Presented at *E-MRS Fall 2021 Meeting*, VIRTUAL, New Mexico, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-28630)

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

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

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

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

Marrone, B. L. BioManufacturing with Intelligent Adaptive Control (BioManIAC). Presented at *American Chemical Society*, Online, New Mexico, United States, 2021-04-05 - 2021-04-30. (LA-UR-21-23378)

Marrone, B. L. BioManufacturing in Cyanobacteria Guided by Intelligent Adaptive Control (BioManIAC). Presented at *International Conference on Algal Biomass, Biofuels, and Bioproducts (AlgalBBB 2021)*, online, New Mexico, United States, 2021-06-14 - 2021-06-16. (LA-UR-21-25535)

Marrone, B. L., C. R. Gonzalez Esquer, C. N. Iverson, P. Patelli, G. Pilania, S. Banerjee, S. N. Twary and R. J. Batrice. Adaptive

Biomanufacturing for CO2 Conversion to Bio-Jet. . (LA-CP-21-20780)

Marrone, B. L., C. R. Gonzalez Esquer and S. M. Van Cuyk. CO2\xc2\xa0Stimulated Algae Growth. Presented at *Visit by Enchant Energy (Virtual)*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-27747)

Marrone, B. L., S. Banerjee and G. Pilania. Predictive Understanding of Harmful Algal Blooms (HABs) using AI Integration of Nutrient, Environment, and 'Omics Information (HAB-AI-NEO). Presented at *Collaborative Opportunities with University of Alaska, Fairbanks, Information Session*, Los Alamos, New Mexico, United States, 2021-08-11 - 2021-08-11. (LA-UR-21-28082)

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

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

Posters

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

Hernandez, M. M., N. S. Gupta, K. Lee, B. L. Marrone, C. N. Iverson and J. H. Dumont. Engineering a Greener Future: Biodegradable Polyhydroxybutyrate Composites. Presented at *American Chemical Society Meeting*, Atlanta, Georgia, United States, 2021-08-23 - 2021-08-23. (LA-UR-21-28590)

Hernandez, M. M., N. S. Gupta, K. Lee, B. L. Marrone, C. N. Iverson and J. H. Dumont. Engineering a Greener Future: Biodegradable Polyhydroxybutyrate Composites. Presented at *American Chemical Society Meeting Fall 2021*, Los Alamos, New Mexico, United States, 2021-08-22 - 2021-08-26. (LA-UR-21-28871)

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

Lalonde, J. N., B. L. Marrone and G. Pilania. A Machine Learning Approach to Investigate Degradation of Poly(hydroxyalkanoates). Presented at *American Association for the Advancement of Science*, Los Alamos, New Mexico, United States, 2021-02-08 - 2021-02-12. (LA-UR-21-30391)

Lalonde, J. N., B. L. Marrone and G. Pilania. A Machine Learning Approach to Investigate Degradation of Poly(hydroxyalkanoates). Presented at *Duke University Center for Biotechnology and Tissue Engineering 2022*

Kewaunee Lecture, Durham, North Carolina, United States, 2022-03-30 - 2022-04-08. (LA-UR-22-22529)

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

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

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Project Description

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

Technical Outcomes

The team quantified metal-containing salt solubility. Data suggest that selective precipitation of specific salts is possible. In-situ characterization using conductance and impedance/dielectric spectroscopy was implemented. Molecular interpretations were guided by both simulation and theory. Specific ions were separated as adducts and insoluble salts. Specific ion removal via binding onto inexpensive minerals was also demonstrated. Oxidization of organics can reduce the cost of fresh water significantly. It appears that supercritical desalination can fulfill its promise.

Publications

Journal Articles

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

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

Messerly, R. A., T. Yoon, R. B. Jadrich, R. P. Currier and K. A. Maerzke. Elucidating the temperature and density dependence of silver chloride hydration numbers in high-temperature water vapor: A first-principles molecular simulation study. 2022. *Chemical Geology*. 120766. (LA-UR-21-29838 DOI: 10.1016/j.chemgeo.2022.120766)

*Middleton, R. S., J. D. Ogland-Hand, B. Chen, J. M. Bielicki, K. M. Ellett, D. R. Harp and R. M. Kammer. Identifying geologic characteristics and operational decisions to meet global carbon sequestration goals. 2020. *Energy & Environmental Science*. **13** (12): 5000-5016. (LA-UR-20-25931 DOI: 10.1039/D0EE02488K)

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

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

Redding, M. R., P. Sharan, T. Yoon and A. T. Findikoglu. Understanding capacitively coupled contactless conductivity detection systems. Submitted to *journal of young investigators*. (LA-UR-21-28813)

Sharan, P., S. Thengene, T. Yoon, R. P. Currier and A. T. Findikoglu. Zero Liquid Discharge for Produced Water Treatment Using Supercritical Desalination Powered by Supercritical Water Oxidation. Submitted to *Desalination*. (LA-UR-21-28816)

*Sharan, P., T. J. Yoon, S. M. Jaffe, T. Ju, R. P. Currier and A. T. Findikoglu. Can capacitive deionization outperform reverse osmosis for brackish water desalination?. 2021. *Cleaner Engineering and Technology*. **3**: 100102. (LA-UR-20-26776 DOI: 10.1016/j.clet.2021.100102)

Sharan, P., T. Yoon, R. P. Currier, R. P. Singh and A. T. Findikoglu. Optimal Design of Multi-Stage Vacuum Membrane Distillation and Integration with Supercritical Water Desalination for Zero Liquid Discharge Desalination. Submitted to *Water Research*. (LA-UR-21-24836)

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

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

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

*Yoon, T. J., L. A. Patel, T. Ju, M. J. Vigil, A. T. Findikoglu, R. P. Currier and K. A. Maerzke. Thermodynamics, dynamics, and structure of supercritical water at extreme conditions. 2020. *Physical Chemistry Chemical Physics*. **22** (28): 16051-16062. (LA-UR-20-22874 DOI: 10.1039/D0CP02288H)

Yoon, T., E. P. Craddock, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Electrical Conductances and association constants in dilute aqueous NdCl 3 solutions from 298 to 523 K along an isobar of 25 MPa. Submitted to *Journal of Chemical & Engineering Data*. (LA-UR-21-30907)

Yoon, T., E. Y. Raby, P. Sharan, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. Electrical characterization of binary mixtures and ternary nanostructured fluids composed of water, 2-propanol, and n-hexane. Submitted to *Journal of Molecular Liquids*. (LA-UR-20-30449)

Yoon, T., J. D. Riglin, P. Sharan, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. An in-situ conductometric apparatus for physicochemical characterization of solutions and in-line monitoring of separation processes at elevated temperatures and pressures. Submitted to *Measurement Science & Technology*. (LA-UR-21-29440)

Yoon, T., K. A. Maerzke, A. T. Findikoglu, R. P. Singh, L. R. Pratt, A. C. Strzelecki, L. A. Patel, D. T. Gomez, R. S. Middleton, C. D. Alcorn, M. J. Vigil, E. Judge, J. D. Riglin, K. A. Velizhanin, R. S. Reid, H. D. Nisbet, A. Migdissov and R. P. Currier. Supercritical Desalination: Opportunities and Challenges. Submitted to *Desalination*. (LA-UR-19-32498)

Yoon, T., K. A. Maerzke, R. P. Currier and A. T. Findikoglu. PyOECP: A flexible open-source software library for estimating and modeling the complex permittivity based on the open-ended coaxial probe (OECP) technique. Submitted to *Computer Physics Communications*. (LA-UR-21-29438)

*Yoon, T., M. J. Vigil, E. Y. Raby, R. P. Singh, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Dielectric relaxation of neodymium chloride in water and in methanol. 2020. *Journal of Molecular Liquids*. **308**: 112981. (LA-UR-19-32739 DOI: 10.1016/j.molliq.2020.112981)

Reports

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

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

Presentation Slides

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

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

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

Maerzke, K. A., L. A. Patel and R. P. Currier. Comparing Classical Force Fields for Aqueous NaCl Solutions at Elevated Temperatures and Pressures. Presented at *21st Symposium on Thermophysical Properties*, Boulder, Colorado, United States, 2021-06-20 - 2021-06-20. (LA-UR-21-25053)

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

Maerzke, K. A., L. A. Patel and T. Yoon. Salts in Hot Water: Developing a Scientific Basis for Supercritical Desalination and Strategic Metal Recovery. . (LA-UR-21-24231)

Maerzke, K. A., R. B. Jadrich, T. Yoon, J. A. Leiding and R. P. Currier. First Principles Simulations of CuCl in High

Temperature Water Vapor. Presented at *Telluride Science Lecture Series*, Los Alamos, New Mexico, United States, 2020-08-07 - 2020-08-07. (LA-UR-20-25990)

Maerzke, K. A., T. Yoon, R. B. Jadrich, J. A. Leiding and R. P. Currier. First Principles Simulations of CuCl in High Temperature Water Vapor. Presented at *21st Symposium on Thermophysical Properties*, Boulder, Colorado, United States, 2021-06-20 - 2021-06-20. (LA-UR-21-24961)

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

Migdissov, A., A. C. Strzelecki, H. Boukhalfa, K. B. Sauer, H. D. Nisbet, K. A. Velizhanin and R. P. Currier. Selective hydrothermal extraction of lanthanides: mimicking natural ore-forming processes. . (LA-UR-20-21659)

Redding, M. R. Understanding Capacitively Coupled Contactless Conductivity Detection Systems. . (LA-UR-21-27098)

Sharan, P., J. Mctigue, T. Yoon, R. P. Currier and A. T. Findikoglu. Reducing the Energy Consumption for Supercritical Water Desalination. Presented at *AGU Fall Meeting 2020*, San Fransisco, California, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29276)

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

Velizhanin, K. A., C. D. Alcorn, A. Migdissov and R. P. Currier. Non-Ideal Solubility of Chlorides in Steam. Presented at *LDRD 20190057DR MidTerm Appraisal*, Los Alamos, New Mexico, United States, 2020-02-24 - 2020-02-24. (LA-UR-20-21646)

Vigil, M. J. Development of Electrochemical Methods for In Situ Diagnostics of Fluids: Impedance Spectroscopy and Cyclic Voltammetry. Presented at *2020 symposium presentation*, Los Alamos, New Mexico, United States, 2020-08-03 - 2020-08-03. (LA-UR-20-25403)

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

Yoon, T., L. A. Patel, M. J. Vigil, A. T. Findikoglu, K. A. Maerzke and R. P. Currier. Molecular dynamics study of specific conductance in sub- and supercritical brine. . (LA-UR-20-21740)

Yoon, T., L. A. Patel, M. J. Vigil, A. T. Findikoglu, K. A. Maerzke and R. P. Currier. Understanding the Specific Conductance of NaCl Solutions in Water at Elevated Temperatures and Pressures. Presented at *2020 Virtual AIChE Annaul Meeting*, Los Alamos, New Mexico, United States, 2020-11-16 - 2020-11-20. (LA-UR-20-28738)

Posters

Patel, L. A. and K. A. Maerzke. NaCl Aggregation in Supercritical Water: Comparison of Classical Force Fields.. . (LA-UR-20-21629)

Redding, M. R., P. Sharan, T. Yoon and A. T. Findikoglu. Understanding Capacitively Coupled Contactless Conductivity Detection Systems. Presented at *ACS Midwest Regional Meeting*, Springfield, Missouri, United States, 2021-10-20 - 2021-10-22. (LA-UR-21-28760)

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

Vigil, M. J., T. Yoon, A. Migdissov, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. Development of Electrochemical Methods for In Situ Diagnostics of Fluids: Impedance Spectroscopy and Cyclic Voltammetry. . (LA-UR-20-26434)

Crucial Radioactive Gas Transport Feedbacks from the Blast Cavity toward the Atmosphere

Philip Stauffer
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Project Description

The international community considers radioactive gases to be a smoking gun for positive identification of subsurface nuclear testing, given the inability of seismic methods to definitively discriminate between chemical and nuclear explosions. However, predicting radioactive gas migration encompasses multiple phenomena, beginning with a nuclear detonation and expanding fireball of gases that rips apart underground facilities, generating far-reaching radial fractures, opening and closing natural fractures, and ultimately injecting gas far into the surrounding rock mass. The current practice for predicting underground nuclear explosion (UNE) gas release uses simplified physics and heuristic validation, resulting in radioactive gas release predictions that are missing key feedbacks that compromise potential future United States (US) test containment or suspected UNEs detection. Similarly, current containment science simulations at Los Alamos National Laboratory and Lawrence Livermore National Laboratory rely on previous generation couplings (e.g., fixed fracture orientations, 2-Dimensional, and continuum approximations) that have limited feedbacks. We aim to reduce uncertainty in gas transport predictions, advancing US national objectives in containment science and underground nuclear explosion detection and characterization.

Technical Outcomes

The team created proof of concept simulations of uncertainty and created new multi-process couplers allowing damage simulations and gas transport simulations to more efficiently pass data. The team used a numerical benchmark to demonstrate that the new coupling scheme is working correctly. The team also built a thermal-hydrological-mechanical-chemical simulation.

Publications

Presentation Slides

Sweeney, M. R., Z. Lei, J. D. Hyman, P. H. Stauffer, J. D. Moulton, K. Lipnikov and D. Svyatsky. Thermo-hydro-mechanical coupling in fracture-matrix systems: meshing, modeling, and applications. Presented at *SIAM Geosciences*, Virtual, Italy, 2021-06-21 - 2021-06-21. (LA-UR-21-25790)

Passive MemComputing in Lithographic Arrays of Interacting Magnetic Nanoislands

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20200105ER

Project Description

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

Publications

Journal Articles

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

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

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

Caravelli, F., M. D. Saccone, K. Hofhuis, S. Parchenko, Y. A. Birkh\xc3\xb6lzer, S. Dhuey, A. K. Kleibert, S. van Dijken, C. Nisoli and A. Farhan. Direct observation of a dynamical glass transition in a nanomagnetic artificial Hopfield network. Submitted to *Nature Physics*. (LA-UR-21-28829)

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

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

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

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

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

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

Hofhuis, K., C. F. Petersen, M. D. Saccone, S. Dhuey, A. Kleibert, S. van Dijken and A. Farhan. Geometrically frustrated kagome-triangular lattice: ice-rule vs. vortex-driven order. Submitted to *Physical Review B*. (LA-UR-21-23310)

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

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

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

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

Saccone, M. D., F. Caravelli, K. Hofhuis, S. Parchenko, S. Dhuey, A. Kleibert, C. Nisoli and A. Farhan. Direct observation of a dynamical glass transition in a nanomagnetic artificial Hopfield network. Submitted to *Nature Physics*. (LA-UR-21-27055)

Saglam, H., C. Nisoli, P. Schiffer and A. Duzgun. Entropy-driven order in an array of nanomagnets. Submitted to *Nature Physics*. (LA-UR-22-21456)

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

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

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

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

Books/Chapters

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

Presentation Slides

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

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

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

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

Posters

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

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

Christina Steadman
20200111ER

Project Description

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

Publications

Journal Articles

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

The Genetic Patterns of Migration in Global Pandemics

Andrey Lokhov
20200121ER

Project Description

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

Publications

Journal Articles

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

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

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

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

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

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

Conference Papers

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

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

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

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

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

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

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

Presentation Slides

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

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

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

Jurgen Schmidt
20200161ER

Project Description

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

Publications

Journal Articles

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

Presentation Slides

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

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

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

Migun Shakya
20200252ER

Project Description

Predicting the effects of climate change is a National and Global Security mission. Understanding carbon (C) cycling in terrestrial ecosystems, which are responsible for ~50% of carbon dioxide (CO_2) emissions, is central to this mission. Accurate models of C flow in Earth systems are pivotal. However, large unexplained variance in C cycle models and poor spatial correlation of predicted and observed terrestrial C stocks create substantial uncertainty in predictions of C cycling. A current focus of model improvement is discovery and inclusion of microbial processes that impact C cycling, where microbes contribute to half (60 gigatonne) of C efflux in the terrestrial biosphere. A major process that has been previously ignored is virus-induced microbial mortality, which is somewhat analogous to insect-driven forest mortality. To inform modeling and ecosystem management, this project will begin to characterize the impact of viruses in driving C cycling dynamics of soil ecosystems.

Publications

Journal Articles

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

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

Viruses. **12** (12): 1424. (LA-UR-20-23300 DOI: 10.3390/v12121424)

Presentation Slides

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

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

Posters

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

Engineering green factories for the production of renewable chemicals

Taraka Dale
20200274ER

Project Description

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

Publications

Presentation Slides

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

Posters

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

Inverse Problem Approach to Spacecraft Charging Simulations

Gian Delzanno
20200276ER

Project Description

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

Publications

Journal Articles

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

*Borovsky, J. E. and G. L. Delzanno. Do Impulsive Solar-Energetic-Electron (SEE) Events Drive High-Voltage Charging Events on the Nightside of the Moon?. 2021. *Frontiers in Astronomy and Space Sciences*. **8**: 655333. (LA-UR-21-20395 DOI: 10.3389/fspas.2021.655333)

. B. J. E. *. H. M. G. *. L. P. A. R. *. R. V. *. W. D. T. Delzanno, G. L., G. L. Delzanno, M. G. Henderson and P. A. R. Lira. The impact of cold electrons and cold ions in magnetospheric physics. 2021. *Journal of Atmospheric and Solar-Terrestrial Physics*. **220: 105599. (LA-UR-20-28089 DOI: 10.1016/j.jastp.2021.105599)

Presentation Slides

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

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

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

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

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

Delzanno, G. L. Space mission concept(s). . (LA-UR-21-26020)

Delzanno, G. L. Advanced modeling in support of space missions. . (LA-UR-21-26164)

Delzanno, G. L. Advanced modeling in support of space missions - part 2 -. . (LA-UR-21-26149)

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

Delzanno, G. L. B-SPICE kick-off: The big picture. . (LA-UR-21-28246)

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

Delzanno, G. L. and J. E. Borovsky. A space mission concept to support the LWS program and space weather: Surveying the cold-electron and cold-ion populations of the magnetosphere for the first time. . (LA-UR-21-26729)

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

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

Godinez Vazquez, H. C., P. A. Resendiz Lira, M. G. Henderson, B. E. Wohlberg and G. L. Delzanno. Environmental and Material Parameter Estimation for Spacecraft Charging Events. Presented at *American Meteorological Society Annual Meeting*, Houston, Texas, United States, 2022-01-24 - 2022-01-28. (LA-UR-22-20699)

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

Posters

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

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

Godinez Vazquez, H. C., P. A. Resendiz Lira, M. G. Henderson, B. E. Wohlberg and G. L. Delzanno. Inverse Approach to Spacecraft Charging Simulations: Parameter Estimation for Material and Space Plasma Environment. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32222)

Nanotherapeutic Adjuvants for Sepsis

Jessica Kubicek-Sutherland
20200300ER

Project Description

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

Publications

Journal Articles

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

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

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

Lenz, K. D., K. E. Klosterman, H. Mukundan and J. Z. Kubicek-Sutherland. A lipoprotein capture ELISA for the detection of amphiphilic biomarkers. Submitted to *Analytical Biochemistry*. (LA-UR-22-22209)

Mansbach, R. A., L. A. Patel, N. A. Watson and S. Gnanakaran. Effects of Sequence on Free Energy Landscapes of \xce\xbc Conotoxins. Submitted to *Journal of Physical Chemistry B*. (LA-UR-21-25634)

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

Books/Chapters

Kubicek-Sutherland, J. Z., D. E. Jacobsen, P. A. Kocheril and Z. R. Stromberg. Biological toxicity and environmental hazards associated with PLGA nanoparticles. (LA-UR-21-32343)

Presentation Slides

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

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

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

Posters

Hiller, M. I., K. D. Lenz, P. A. Kocheril, D. E. Jacobsen, C. A. Lopez Bautista, S. Gnanakaran and J. Z. Kubicek-Sutherland. Formulation and Screening of Synthetic Lipoproteins for Binding and Inhibition of Endotoxin.. Presented at *Biophysical Society Annual Meeting*, San Francisco,

California, United States, 2022-02-19 - 2022-02-23. (LA-UR-22-20953)

Klosterman, K. E., K. D. Lenz, H. Mukundan and J. Z. Kubicek-Sutherland. BIOPHYSICAL CHARACTERIZATION OF HUMAN LIPOPROTEINS FOR DIAGNOSTIC ASSAY DEVELOPMENT. Presented at *Biophysical Society Annual Meeting 2021*, Virtual, New Mexico, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-20305)

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

Particle Modeling of High-Altitude Nuclear Explosions

Ari Le
20200334ER

Project Description

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

Publications

Journal Articles

Dorst, R., D. B. Schaeffer, A. Y. Le, J. J. Pilgram, C. G. Constantin, S. Vincena, S. K. Tripathi, D. Winske, D. Larson, M. Cowee and C. Niemann. Planar Laser Induced Fluorescence Mapping of a Carbon Laser Produced Plasma. Submitted to *Physics of Plasmas*. (LA-UR-22-21403)

Keenan, B., A. Y. Le, D. Winske, A. J. Stanier, B. A. Wetherton, M. Cowee and F. Guo. Hybrid particle-in-cell simulations of electromagnetic coupling and waves from streaming burst debris. 2022. *Physics of Plasmas*. **29** (1): 012107. (LA-UR-21-29875 DOI: 10.1063/5.0075482)

*Le, A. Y., D. Winske, A. J. Stanier, W. S. Daughton, M. Cowee, B. A. Wetherton and F. Guo. Astrophysical Explosions Revisited: Collisionless Coupling of Debris to Magnetized Plasma. 2021. *Journal of Geophysical Research: Space Physics*. **126** (9): e2021JA029125. (LA-UR-20-30244 DOI: 10.1029/2021JA029125)

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

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

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

Reports

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

Presentation Slides

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

Le, A. Y., B. A. Wetherton, J. Egedal, C. B. Forest, W. S. Daughton and A. J. Stanier. End Losses from a Magnetic Mirror: Kinetic Simulations and Guiding Center Theory. Presented at *APS Division of Plasma Physics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-28879)

Le, A. Y., B. Keenan, D. Winske, A. J. Stanier, B. A. Wetherton, F. Guo and M. Cowee. Explosion Debris-Driven Electromagnetic Ion-Ion Beam Instabilities. Presented at *APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30899)

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

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

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

Le, A. Y., V. Roytershteyn, H. Karimabadi, A. J. Stanier, L. Chacon and K. Schneider. Wavelet Methods for Studying the Onset of Strong Plasma Turbulence. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-09. (LA-UR-20-21673)

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

Posters

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

Capturing the First Uranium Alkylidene Complex

Jaqueline Kiplinger
20200338ER

Project Description

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

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

Karissa Sanbonmatsu
20210134ER

Project Description

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

Publications

Journal Articles

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

Books/Chapters

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

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

Jonathan Schwenk
20210213ER

Project Description

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

Publications

Journal Articles

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

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

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

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

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

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

Reports

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

Presentation Slides

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

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

Schwenk, J. P. and J. Hariharan. Exploring river and delta channel networks with RivGraph. Presented at *Community Surface Dynamics Modeling System Annual Meeting*,

Boulder, Colorado, United States, 2021-05-20 - 2021-05-20. (LA-UR-21-30437)

Posters

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

Other

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

Local Transition Modeling for Mixing

Daniel Israel
20210218ER

Project Description

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

Publications

Presentation Slides

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

Grid Scale Energy Storage Using Hydrazine Produced from Lanthanide Electrocatalysis

Benjamin Davis
20210251ER

Project Description

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

Publications

Presentation Slides

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

Other

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

Blurring the Lines Between Ocean Parameterization and Large Eddy Simulation

Luke Van Roekel
20210289ER

Project Description

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

Publications

Journal Articles

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

Presentation Slides

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

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

New Possibilities and Discovery Methods for Explosives Synthesis and Formulation

William Perry
20210339ER

Project Description

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

Publications

Journal Articles

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

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

Walters, D. O., O. Sen, N. K. Rai and W. L. Perry. Toward a machine-guided approach to energetic material discovery. Submitted to *Journal of Applied Physics*. (LA-UR-21-31595)

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

Michael Henderson
20210440ER

Project Description

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

Publications

Journal Articles

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

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

Henderson, M. G. Association of Meso-Scale Auroral Structures and Pseudo-Breakups with Energetic Particle Injections at Geosynchronous Orbit. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-21-27729)

Posters

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

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

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

Matthew Belobrajdic
20210724ER

Project Description

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

Terbium-161 for targeted radionuclide therapy

Veronika Mocko
20210842ER

Project Description

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

Identifying Viral Variants of Concern in a World of Noisy Evolution

Emma Goldberg
20210887ER

Project Description

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

Publications

Journal Articles

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

Visualizing and Understanding Complex Fluid Transport in 3-Dimensional Microstructure

Hari Viswanathan
20180151ER

Project Description

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

Technical Outcomes

For many subsurface energy applications, particles called proppants are introduced into the flow to prop open fractures and play a critical role in optimizing hydrocarbon or heat extraction in hydraulic fracturing and geothermal operations. We integrated cutting edge fluid flow simulation with state of the art Los Alamos three dimensional experimental particle tracking methods to characterize complex fluid and particle transport in fractured media with the aim to optimize proppant dispersal within a fracture network.

Publications

Journal Articles

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

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

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

*Mehana, M., S. A. Hosseini, T. A. Meckel and H. Viswanathan. Modeling CO2 plume migration using an invasion-percolation approach that includes dissolution. 2020. *Greenhouse Gases: Science and Technology*. **10** (2): 283-295. (LA-UR-19-26910 DOI: 10.1002/ghg.1976)

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

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

*Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, J. Carmeliet and D. Derome. Three influential factors on colloidal nanoparticle deposition for heat conduction enhancement in 3D chip stacks. 2021. *Applied Thermal Engineering*. **187**: 116585. (LA-UR-20-23176 DOI: 10.1016/j.applthermaleng.2021.116585)

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

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

Presentation Slides

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Posters

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

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

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

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

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

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

Other

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

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

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

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

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

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

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

In Situ Characterization of Uranium Hydriding Corrosion

Terry Holesinger
20180295ER

Project Description

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

Technical Outcomes

The project successfully used post mortem characterization of existing hydride structures to gain new insights on structures and potential situations under which they may form. This data was used in theory development and modeling to show that one proposed nucleation site, twin boundaries, are plausible locations at which nucleation could occur. The team was unsuccessful in the final objective of directly observing hydride nucleation and growth due to COVID and limited facility availability.

Publications

Journal Articles

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

Reports

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

Presentation Slides

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

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

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

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

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

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, M. A. Hill, E. L. Tegtmeier, S. K. Lawrence, R. K. Schulze and A. W. Richards. Early Stage Uranium Hydride Development in Cast U238. Presented at *Presentation to external agency*,

Reading, United Kingdom, 2020-02-12 - 2020-02-14. (LA-UR-20-20934)

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

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

Posters

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, R. K. Schulze, E. L. Tegtmeier and A. W. Richards. Towards Understanding the Atomistic to Mesoscopic Processes in Uranium Hydride Nucleation and Growth. Presented at *Pu Futures - The Science 2018*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28414)

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

Chemistry of a New Oxidation State for the Early Transuranic Elements

Andrew Gaunt
20190091ER

Project Description

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

Technical Outcomes

The project was successful in understanding the role of the 5f-electrons in compounds and elucidating the chemical bonding of the actinide elements. This project maintained Los Alamos as the world leader in inert atmosphere transuranium molecular chemistry. The team reported the first structurally authenticated Americium-Carbon (Am-C) bond and only the second ever verified Neptunium(np) (II) + complex, a number of rare Np organometallic molecules, pioneering tracer studies to follow divalent accessibility.

Publications

Journal Articles

P. Goodwin, C. A., A. W. Schlimgen, T. E. Albrecht-Sch \xc3\xb6nzart, E. R. Batista, A. J. Gaunt, M. T. Janicke, S. A. Kozimor, B. L. Scott, L. M. Stevens, F. D. J. White and P. Yang. Structural and Spectroscopic Comparison of Soft-Se vs. Hard-O Donor Bonding in Trivalent Americium/Neodymium Molecules. 2021. *Angewandte Chemie International Edition*. **60** (17): 9459-9466. (LA-UR-21-20831 DOI: 10.1002/anie.202017186)

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

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

P. Goodwin, C. A., S. R. Ciccone, S. Bekoe, S. Majumdar, B. L. Scott, J. W. Ziller, A. J. Gaunt, F. Furche and W. J. Evans. 2.2.2-Cryptand Complexes of Neptunium(III) and Plutonium(III). Submitted to *Angewandte Chemie - International Edition*. (LA-UR-21-27533)

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

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

Reports

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

Presentation Slides

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

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

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

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

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

Stevens, L. M. Elucidation of Electronic Structure and Bonding in Organometallic Actinide Complexes. Presented at *American Chemical Society Fall 2021 Meeting and Exposition*, Atlanta, Georgia, United States, 2021-08-22 - 2021-08-26. (LA-UR-21-28143)

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

Posters

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

Understanding and Predicting Hydrocarbon Behaviors in Nanopores of Tight Reservoirs

Qinjun Kang
20190153ER

Project Description

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

Technical Outcomes

This project successfully addressed the fundamental problems underlying low recovery rates of unconventional oil/gas productions, and achieved the goal to improve our understanding and prediction of hydrocarbon mobility and phase behavior in nanopores of tight formations. The knowledge and fundamental understanding gained from this research can provide critical information to improve reservoir engineering processes in tight oil/gas development, and can also contribute to other mission-critical areas such as carbon dioxide sequestration and enhanced geothermal systems.

Publications

Journal Articles

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

Fang, C., Q. Kang and R. Qiao. The Role of Disjoining Pressure and Thermal Activation in the Invasion of Droplets into Nanopores. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-20142)

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

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

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

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

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

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

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

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

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

*Mehana, M., S. A. Hosseini, T. A. Meckel and H. Viswanathan. Modeling CO2 plume migration using an invasion-percolation approach that includes dissolution. 2020. *Greenhouse Gases: Science and Technology*. **10** (2): 283-295. (LA-UR-19-26910 DOI: 10.1002/ghg.1976)

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

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

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

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

Neil, C. W., R. P. J. Hjelm, M. E. Hawley, E. B. Watkins, C. B. Cockreham, D. Wu, Y. Mao, M. C. Cheshire, J. Burger, T. Fischer, M. R. Stokes and H. Xu. Probing Oil Recovery in Shale Nanopores with Small-Angle and Ultra-Small-Neutron Scattering. Submitted to *International Journal of Coal Geology*. (LA-UR-21-26696)

Qin, F., J. Zhao, Q. Kang, D. Derome and J. Carmeliet. Lattice Boltzmann Modeling of Drying of Porous Media Considering Contact Angle Hysteresis. 2021. *Transport in Porous Media*. (LA-UR-21-21975 DOI: 10.1007/s11242-021-01644-9)

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

*Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, J. Carmeliet and D. Derome. Three influential factors on colloidal nanoparticle deposition for heat conduction enhancement in 3D chip stacks. 2021. *Applied Thermal Engineering*. **187**: 116585. (LA-UR-20-23176 DOI: 10.1016/j.applthermaleng.2021.116585)

*Qin, F., M. Su, J. Zhao, A. Mazloomi Moqaddam, L. D. Carro, T. Brunschwiler, Q. Kang, Y. Song, D. Derome and J. Carmeliet. Controlled 3D nanoparticle deposition by drying of colloidal suspension in designed thin micro-porous architectures. 2020. *International Journal of Heat and Mass Transfer*. **158**: 120000. (LA-UR-19-31518 DOI: 10.1016/j.ijheatmasstransfer.2020.120000)

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

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

*Zhao, J., F. Qin, D. Derome, Q. Kang and J. Carmeliet. Improved pore network models to simulate single-phase flow in porous media by coupling with lattice Boltzmann method. 2020. *Advances in Water Resources*. **145**: 103738. (LA-UR-20-21321 DOI: 10.1016/j.advwatres.2020.103738)

Zhao, J., F. Qin, Q. Kang, C. Qin, D. Derome and J. Carmeliet. A dynamic pore network model for imbibition simulation considering corner film flow. Submitted to *Water Resources Research*. (LA-UR-21-32185)

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

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

Conference Papers

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

S. Mehana, M. Z., J. W. Carey, G. D. J. Guthrie, J. D. Hyman, Q. Kang, S. Karra, C. W. Neil, M. R. Sweeney, H. Xu, H.

S. Viswanathan and J. Santos. Discovery Science of Hydraulic Fracturing and Shale Fundamentals. Presented at *Unconventional Resources Technology Conference*. (Houston, Texas, United States, 2021-07-26 - 2021-07-28). (LA-UR-21-25369)

Books/Chapters

Wang, J., F. Qin, J. Zhao, L. Chen and Q. Kang. Pore-scale simulations and digital rock physics. (LA-UR-21-27732)

Presentation Slides

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

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

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

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

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

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

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

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

Kang, Q. LBM3RT Simulation of Reactive Transport in Porous Media. . (LA-UR-21-25721)

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

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

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

S. Mehana, M. Z. Data-driven Models of Adsorption Equilibria of Multi-component Mixtures in Porous Materials. Presented at *ISTI review*, Los alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-29091)

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

Posters

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

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

Other

S. Mehana, M. Z. Dataset for Machine learning summer school. Dataset. (LA-UR-21-26705)

Using Solar Energetic Protons to Monitor the Outer Magnetosphere

Steven Morley
20190262ER

Project Description

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

Technical Outcomes

The team developed and released a simulation code to predict the access of solar energetic particles in the magnetosphere. The predictions were compared with measurements from particle detectors on the Global Positioning System satellites, thereby quantifying the performance of empirical magnetic field models. Comprehensive analyses of the science and engineering capability of the Global Positioning System particle detectors has been published. A preliminary predictive model of solar energetic particle access was developed.

Publications

Journal Articles

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

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

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

Hendry, A., C. J. Rodger, M. Cliverd and S. K. Morley. Evidence of sub-MeV EMIC-driven trapped electron flux dropouts from GPS observations. Submitted to *Geophysical Research Letters*. (LA-UR-21-24234)

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

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

Olifer, L., S. K. Morley, L. G. Ozeke, I. R. Mann, M. Kalliokoski, M. G. Henderson, R. A. Niyazov and A. S. Hoover. Rapid Acceleration Bursts in the Van Allen Radiation Belt. Submitted to *Nature Physics*. (LA-UR-21-31391)

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

Rodger, C. J., A. T. Hendry, M. A. Cliverd, C. Forsyth and S. K. Morley. Examination of Radiation Belt Dynamics during Substorm Clusters: Activity, Drivers and Dependencies of Trapped Flux Enhancements. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-21-30138)

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

. M. S. K. *. W. C. E. J. *. B. S. N. *. W. P. D. Thompson, R. L. and S. K. Morley. Pro- * - A Probabilistic * Mapping Tool for Ground Observations. 2020. *Space Weather*. **19 (2): e2020SW002602. (LA-UR-20-25802 DOI: 10.1029/2020SW002602)

Conference Papers

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

Reports

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

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

Presentation Slides

Carver, M. R., S. K. Morley and A. L. Stricklan. GPS Constellation Energetic Particle Measurements. Presented at *IEEE Aerospace*, Big Sky, Montana, United States, 2020-03-07 - 2020-03-14. (LA-UR-20-22719)

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

Chen, Y., S. K. Morley and A. S. Hoover. Reproducing Temporal Profiles of Solar Energetic Proton Fluxes in Well-connected Events. Presented at *AGU Fall meeting 2021*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-27584)

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

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

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

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

Olifer, L. and S. K. Morley. Revealing Very Fast Non-Adiabatic Radiation Belt Dynamics With the GPS Constellation. . (LA-UR-21-27866)

Posters

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

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

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

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

Innovating Wildfire Representation in Earth System Models (ESMs)

Alexandra Jonko
20190310ER

Project Description

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

Technical Outcomes

The project used a combination of fine-scale datasets of vegetation and topography and LANL's fire behavior model to characterize the California landscape and produce an ensemble of representative simulations. Both were used to build a statistical model of fire spread, producing improved estimates of wildfire burned area at the Earth System Model grid scale. In addition, the project enabled the development of QUIC-Fire, RD100 winning fire prediction software.

Publications

Journal Articles

Bennett, K. E., A. Jonko, A. Hanbury-Brown, J. A. Oliveto and L. M. Kueppers. Title: Impacts of multiple burns on post-fire vegetation recovery in California. Submitted to *Environmental Research Letters*. (LA-UR-21-29596)

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

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

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

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

Zhai, L., D. R. Coyle, D. Li and A. Jonko. Fire, insect, and disease-caused tree mortalities increased in forests of greater structural diversity during drought. Submitted to *Journal of Ecology*. (LA-UR-21-28195)

Reports

Oliveto, J. A. and A. Jonko. Studying Rate of Fire Spread Using Landscape Statistics and FIRETEC. Unpublished report. (LA-UR-21-29598)

Presentation Slides

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

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

Jonko, A. California Ecosystem Futures Meeting LANL Update. Presented at *UC Fees California Ecosystem Futures Semi Annual Meeting*, Virtual, California, United States, 2021-04-29 - 2021-04-30. (LA-UR-21-24150)

Jonko, A., K. E. Bennett, R. R. Linn, J. A. Oliveto and D. R. Livingston. Incorporating effects of topography and subgrid-scale vegetation heterogeneity on fire spread into Earth System Models. Presented at *"California Ecosystem*

Futures" UC Lab Fees Project Meeting, Los Alamos, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-21308)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Illuminating Plutonium: Spectroelectrochemisty in High Temperature Molten Salts

Benjamin Stein
20190364ER

Project Description

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

Technical Outcomes

This project advanced understanding of actinides in molten salts and spurred follow-on work. Specifically, the team developed instrumentation that allows to to monitor the speciation of plutonium and other elements of interest (e.g. uranium and americium) as well as theoretical methods to treat the same.

Publications

Journal Articles

MacInnes, M. M., Z. R. Jones, N. H. Anderson, C. Eiroa Lledo, M. Y. Livshits, S. A. Kozimor, V. Mocko, F. Rein Rocha, B. Stein, K. E. Knope and J. N. Wacker. Using Molten Salts to Probe Outer-Coordination Sphere Effects on Lanthanide(III/II) Electron-Transfer Reactions. Submitted to *Journal of the American Chemical Society*. (LA-UR-21-25246)

Reports

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

Presentation Slides

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

Biogenic Uranium Isotope Fractionation for Biotechnology

Robert Williams
20190372ER

Project Description

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

Technical Outcomes

The team accomplished all of the technical goals to characterize uranyl bioreduction controlling uranium isotope fractionation. Controlled anaerobic cellular growth was achieved; however, measuring uranium isotopes in the microbial lysate required significant methods development. Confirmation using the Laboratory's Thermal Ionization Mass Spectrometry Facility provided the first measurements of uranium bioreduction and a true isotopic mass balance in cells. Multi-step fractionation processes are complex, but these results show promise for enrichment based on cellular bioaccumulation mechanisms.

Publications

Journal Articles

Gonzalez, J. M., R. Marti-Arbona, J. C. Chen and C. J. UNkefer. Binding plasticity of phosphoenolpyruvate revealed by the structure of Synechococcus elongatus enolase. Submitted to *Acta Crystallographica. Section F: Structural Biology Communications*. (LA-UR-22-20772)

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

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

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

Reports

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

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

Presentation Slides

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

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

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

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

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

Posters

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

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

Kshitij Wagh
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Project Description

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

Technical Outcomes

The team successfully developed a coarse-grained strategy to enable efficient long time scale simulation of dynamics of large glycan-protein systems, and applied this to obtain glycan dynamics for 13 HIV strains using experimental glycan heterogeneity data. The team also developed novel high throughput machine learning strategies using sequence features to accurately predict HIV glycan shield and glycan heterogeneity. The team investigated the structural relevance of SARS-

CoV-2 Alpha variant Spike mutations for resistance to therapeutic antibodies.

Publications

Journal Articles

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

Gnanakaran, S., S. Welbourn, S. Chakraborty, J. E. Yang, A. S. Gleinich, S. Gangadhara, S. Khan, C. Ferrebee, B. Yagnik, S. Burton, T. Charles, S. A. Smith, D. Williams, R. Mopuri, A. A. Upadhyay, J. Thompson, M. A. Price, S. Wang, Z. Qin, X. Shen, L. D. Williams, N. Eisel, T. Peters, L. Zhang, W. Kilembe, E. Karita, G. D. Tomaras, S. E. Bosinger, R. R. Amara, P. Azadi, E. R. Wright and C. A. Derdeyn. A neutralizing antibody target in early HIV-1 infection was recapitulated in rhesus macaques immunized with the transmitted/founder envelope sequence. Submitted to *PLOS Pathogens*. (LA-UR-22-22584)

*T. H. *. M. C. *. W. K. *. F. W. *. T. J. *. Y. H. *. L. D. *. H. B. F. *. S. K. O. *. G. S. *. H. N. *. P. R. *. S. G. *. G. G. M. *. K. B. *. M. D. C. Shen, X. *., K. Wagh, H. Yoon, S. Gnanakaran, W. Fischer, J. Theiler, N. Hengartner and B. Korber. SARS-CoV-2 variant B.1.1.7 is susceptible to neutralizing antibodies elicited by ancestral spike vaccines. 2021. *Cell Host & Microbe*. **29** (4): 529-539. (LA-UR-21-20697 DOI: 10.1016/j.chom.2021.03.002)

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

Wagh, K., B. T. M. Korber, F. Cai, W. Chen, W. Wu, J. Jones, M. Choe, N. Gohain, X. Shen, C. Labranche, A. Eaton, L. Sutherland, G. Hernandez, N. R. Wu, R. M. Scearce, M. S. Seaman, M. A. Moody, S. Santra, K. Wiehe, G. D. Tomaras, M. Bonsignori, D. Montefiori, B. F. Haynes, N. de Val, M. G. Joyce and K. O. Saunders. HIV-1 vaccination elicits structurally and genetically-convergent neutralizing antibodies in non-human primates. Submitted to *PLOS Pathogens*. (LA-UR-21-29267)

Presentation Slides

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

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

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

Michael Fassbender
20200165ER

Project Description

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

Technical Outcomes

A small millifluidic device was designed that produces radiopharmaceuticals for cancer treatment. It was manufactured via three-dimensional printing using a resin with high chemical and radiation stability. Unique features of the device are small fluidic channels that were printed down to 1 millimeter diameter. The centerpiece of the device is an electrochemical radioisotope generator that generates short-lived alpha emitter Bismuth-213; this isotope is then immediately attached to antibodies to irradiate malignant cells inside the human body.

Publications

Reports

H. Dutech, G. R., A. C. Akin, A. N. Marchi, K. A. Lopez, K. N. Husmann, M. E. Fassbender, E. J. O'Donnell, T. Mastren and R. Forrester. 225Ac/213Bi Generator Based on Millifluidics Controlled Electrodeposition. Unpublished report. (LA-UR-21-32345)

Fassbender, M. E. 225Ac/213Bi Generator Based on Millifluidics Controlled Electrodeposition. Unpublished report. (LA-UR-21-29374)

Posters

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

Next Steps to Molecular Actinide Nitrides

Marisa Monreal
20200435ER

Project Description

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

Technical Outcomes

This project's technical outcomes addressed the high-level goal of of contributing to the understanding of the chemical behavior of nuclear fuels. The electrochemical system required to study organometallic molecules using electrochemical techniques was advanced and optimized, and this system may be used to study a set of organometallic molecules including those with relevance to accident-tolerant nuclear fuels. An unexpected achievement during the course of this research was the design of a new type of electrode.

Universal first response countermeasures for current and future pandemic threats: Broad Spectrum Antivirals targeting Host Proteins

Jurgen Schmidt
20210705ER

Project Description

There exist an estimated 10^31 viruses on Earth, far more than planets in the universe. While only few of those are threats of human concern, the number of potential pandemic causing species and variants among viral families remains staggering. As the current coronavirus (Covid) pandemic demonstrates, we are woefully unprepared for emerging challenges. Currently, the vast majority of antiviral drug design efforts target specific viral proteins on specific viruses. In addition, vaccine efforts are highly specific to the viral threat present. These strategies are retroactive, time consuming and generally cannot prepare for the next, unknown pandemic. All viruses have one potential Achilles heel in common; they need to interact with the host to invade cells, counter host defenses and replicate. We propose a novel, general strategy, shifting the focus to target human host proteins essential for viral entry and replication. We will develop strategies to hinder and slow viral host cell interactions in the initial stages of infection affording the host the necessary time to mount an immune response. We suggest that this provides pan viral and universal "off the shelf" first response countermeasures against both naturally emerging and man-made viral biothreats.

Technical Outcomes

The project demonstrated that epitope regions of viral proteins that interact with the host cell in the initial phase of infection can be readily and rapidly identified by molecular simulations, such epitopes reduced to peptides and peptide mimetic motives can be readily synthesized to afford inhibitors broadly active against viral families and mutational variants.

Publications

Journal Articles

Schmidt, J. G., C. H. Schein, G. Rafael, W. S. Baker, E. S. Anaya, S. C. Weaver, S. Negi and W. Braun. Exclusivity versus promiscuity in the immune response to PCP-consensus, alphavirus antigens. Submitted to *Vaccine*. (LA-UR-21-31370)

REECoVER: Recovering Critical Rare Earth Elements (REEs) and Cobalt (Co) from End-of-Life Permanent Magnet Waste

Jaqueline Kiplinger
20210707ER

Project Description

Rare-earth element (REE) based neodymium-iron-boron(dysprosium) (Nd-Fe-B(Dy) and samarium-cobalt (Sm-Co) permanent magnets have been widely used because of their excellent magnetic properties. Significant amounts of Nd-Fe-B(Dy) and Sm-Co magnets are found in consumer, industrial, and military defense products, providing a potential secondary supply of these metals. Although recycling these magnets can lower the supply risk of Nd, Dy, Sm, and Co, only very small quantities of REE (~ 1%) have been recycled from pre-consumer scrap, and the United States (US) is completely dependent on imports for its supply of Co. At present, no commercial operation has been identified for recycling the end-of-life Nd-Fe-B or Sm-Co permanent magnets and the recovery of the associated REE content. To address this technology gap, we propose a new Los Alamos National Laboratory (LANL) recycling strategy, REECoVER - for recovering (1) Nd and Dy, and (2) Sm and Co, from scrap and used Nd-Fe-B(Dy) and Sm-Co permanent magnets, respectively - which stands to reduce the US dependence on foreign Nation's for these critical materials.

Technical Outcomes

A transformational green chemistry process - REECoVER - for the recovery of rare earth elements (REE, critical materials) from common commercial/scrap REE permanent magnets was developed. High visibility signature results include the selective removal and recovery of neodymium (Nd) and dysprosium (Dy) from neodymium-iron-boron (Nd-Fe-B) magnets in the form of rare earth chlorides as the final product. The postdoctoral research this one year project supported has contributed to three manuscripts from efforts on this project.

Electric Field Swing Adsorption - A Process Intensification Tool For Selective Removal of Specific Molecules

John Gordon
20210708ER

Project Description

Our hypothesis-driven science, goals, and objectives advance the Department of Energy (DOE) mission in energy, environment, and national security. LDRD supported research includes an emphasis on discovery, design, and understanding of new materials and chemical processes. Our efforts outlined herein will help define a path forward in the design, testing and evaluation of new field-activated adsorbents capable of selectively sequestering and releasing carbon dioxide (CO_2). Other ramifications of this effort are evident. For example, in addition to CO_2 capture from the air and from flue gases (e.g. at conventional power plants), this approach can also form the basis for capturing toxins and environmentally hazardous trace gases from stack (exhaust) gases, thus we anticipate it will also find applications in limiting on-site emissions. It may also prove effective in dewatering applications (e.g. drying of natural gas or removal of hydrogen dioxide (H_2O) from air in arid climates, where such a resource is precious). Other potential applications include the adsorption and subsequent conversion of adsorbed CO_2 into industrially relevant chemicals.

Technical Outcomes

The team learned that high field strengths, likely to induce dielectric breakdown, will be needed to significantly impact carbon dioxide (CO_2) adsorption. A revised hypothesis that has resulted, is that externally applied E-fields can be used to enhance thermally driven CO_2 reactivity and conversion chemistry. Recent reports appear to support such field-enhanced catalysis. E-field enhancement has not been applied to CO_2 reactions; Los Alamos is now positioned to assume the lead in doing this.

Electromagnetic Pulse (EMP) Impacts On Telecommunication Networks

Michael Rivera
20210710ER

Project Description

The proposed work directly addresses Department of Energy (DOE) and Department of Homeland Security (DHS) requirements put forth in the recent electromagnetic pulse (EMP) executive order with regards to the evaluation of EMP impacts to critical infrastructure systems. In particular, the proposed research addresses the problem of how to evaluate EMP impacts to telecommunication infrastructure which impacts both the telecommunication critical infrastructure network as well as the power delivery network which uses telecommunication components to control power delivery systems.

Technical Outcomes

The project developed a network and demand generation tool using open sources of data and the location of existent infrastructure to estimate physical locations of network elements and traffic demand patterns. Traffic flow within this network was estimated by implementing a minimum delay traffic algorithm that produces a lower bound estimate of packet congestion within the network. An undisturbed network flow pattern was produced, as was a flow pattern following an electromagnetic pulse insult.

Publications

Journal Articles

Boero, R. and M. K. Rivera. Estimation of IP Traffic Matrices based on Internet Service Supply and Demand. Submitted to *Journal of Infrastructure Systems*. (LA-UR-21-31714)

Quantification and Modelling of Immune Responses to Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) Infection

Carmen Molina-Paris
20210730ER

Project Description

Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) is responsible for the pandemic of greatest human and economic impact in the past 100 years. It is now clear that only a safe and protective vaccine will curb this pandemic and allow us to return to ``normal'' life. What immune mechanisms make a vaccine protective, when does an individual develop immune protection after vaccination, or how long will vaccine immunity last are questions that require immediate answers. In this proposal, we will quantify the dynamics of SARS-CoV-2 immune responses using mathematical models, together with clinical and experimental data, to address those timely questions. This project can have an important impact on the Department of Energy's mission of ``Science & innovation'', especially regarding national security, by improving our knowledge and capabilities to control this pandemic. The results of this project can be integrated in population-level models to better predict the epidemiological spread of infection. The project will also keep Los Alamos National Laboratory at the forefront of research in this area.

Technical Outcomes

The team analysed viral load dynamics in different anatomic compartments in hospitalized individuals with COVID-19 and the effect of remdesivir treatment on viral kinetics. Analysis of the St. Jude data set supports the observation that post-vaccine levels of antibodies for the receptor-binding-domain and spike protein of SARS-CoV-2 are larger than those induced by infection. Our results indicate significant (and unexpected) correlations between common cold coronavirus basal antibody levels and those induced by the SARS-CoV-2 vaccine.

Publications

Journal Articles

Prevalence of SARS-CoV-2 Antibodies after First 6 Months of COVID-19 Pandemic, Portugal. 2021. *Emerging Infectious Diseases*. **27** (11): 2878-2881. (LA-UR-21-22054 DOI: 10.3201/eid2711.210636)

Canto e Castro, L., A. Gomes, M. Serrano, A. H. Guia Pereira, R. Ribeiro, P. Napole\xc3\xa3o, I. Domingues, C. Silva, J. Fanczal, \. Afonso, A. Lopes, I. Toader, M. J. Rego de Sousa, J. G. Rego de Sousa, G. de Sousa, M. M. Mota, B. Silva-Santos, M. Veldhoen and R. M. Ribeiro. Longitudinal SARS-CoV-2 seroprevalence in Portugal and antibody maintenance 12 months after the start of the COVID-19 pandemic. Submitted to *Nature Communications*. (LA-UR-21-25341)

Chew, K. W., C. Moser, E. S. Daar, D. A. Wohl, J. Z. Li, R. Coombs, J. Ritz, M. Giganti, A. C. Javan, Y. Li, C. Malvestutto, P. Klekotka, K. Price, A. Nirula, W. Fischer, V. Bala, R. M. Ribeiro, A. S. Perelson, C. V. Fletcher, J. J. Eron, J. S. Currier, M. D. Hughes and D. M. Smith. Bamlanivimab reduces nasopharyngeal SARS-CoV-2 RNA levels but not symptom duration in non-hospitalized adults with COVID-19. Submitted to *Nature Microbiology*. (LA-UR-22-20405)

Choudhary, M. C., K. W. Chew, R. Deo, J. P. Flynn, J. Regan, C. R. Crain, C. Moser, M. Hughes, J. Ritz, R. M. Ribeiro, R. Ke, J. A. Dragavon, A. C. Javan, A. Nirula, P. Klekotka, A. L. Greninger, C. V. Fletcher, E. S. Daar, D. A. Wohl, J. J. Eron, J. S. Currier, U. M. Parikh, S. F. Sieg, A. S. Perelson, R. W. Coombs, D. M. Smith and J. Z. Li. Emergence of SARS-CoV-2 Resistance with Monoclonal Antibody Therapy. Submitted to *Nature*. (LA-UR-21-27556)

Gaevert, J. A., D. Luque Duque, G. Lythe, C. Molina-Paris and P. G. Thomas. Quantifying cross-reactivity: influenza and coronaviruses. Submitted to *Viruses*. (LA-UR-21-26082)

Ke, R., C. Zitzmann, D. D. Ho, R. M. Ribeiro and A. S. Perelson. In vivo kinetics of SARS-CoV-2 infection and its relationship with a person's infectiousness. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-21-26047)

McGargill, M. A., C. St. Jude and C. Molina-Paris. Pre-existing humoral immunity to common human coronaviruses negatively impacts the protective SARS-CoV-2 antibody response.. Submitted to *Cell Host & Microbe*. (LA-UR-21-30006)

*Regan, J., J. P. Flynn, A. Rosenthal, H. Jordan, Y. Li, R. Chishti, F. Giguel, H. Corry, K. Coxen, J. Fajnzylber, E. Gillespie, D.

R. Kuritzkes, N. Hacohen, M. B. Goldberg, M. R. Filbin, X. G. Yu, L. Baden, R. M. Ribeiro, A. S. Perelson, J. M. Conway and J. Z. Li. Viral Load Kinetics of Severe Acute Respiratory Syndrome Coronavirus 2 in Hospitalized Individuals With Coronavirus Disease 2019. 2021. *Open Forum Infectious Diseases*. **8** (8): ofab153. (LA-UR-21-22010 DOI: 10.1093/ofid/ofab153)

Conference Papers

Lythe, G., R. Callard, R. Hoare and C. Molina-Paris. How many T~cell receptor clonotypes does a body maintain? a stochastic mathematical approach/study. Presented at *Los Alamos -- Arizona Days*. (Los Alamos, New Mexico, United States, 2021-05-18 - 2021-05-18). (LA-UR-21-24749)

Reports

Molina-Paris, C., D. Luque Duque, G. D. Lythe and M. Lopez-Garcia. Multivariate competition for survival stimulus of T cell clonotypes in homeostasis. Unpublished report. (LA-UR-21-21133)

Presentation Slides

Luque Duque, D., E. Stirk, H. van den Berg, M. Lopez-Garcia, G. Lythe and C. Molina-Paris. A stochastic story of the naive T cell population: size, diversity and cross-reactivity. . (LA-UR-22-22089)

Molina-Paris, C., G. Lythe, C. Taylor, M. Locke, D. Luque Duque, P. Thomas and J. Gaevert. St Jude SARS-CoV-2 statistical analysis. . (LA-UR-21-25598)

Modeling the Transport of Compressible Fluids Through Human Engineered Environments at Scale and their Interactions with Natural Environments

Russell Bent
20210778ER

Project Description

By advancing and synthesizing the leading models for subsurface compressible fluid flow, compressible fluid transport through human engineered pipeline systems, and contemporary optimization methods, this project proposes to build new decision support capability for Carbon Capture and Storage (CCS). We aim to bridge fundamental gaps in state-of-the-art CCS modeling and simulation, in particular by incorporating detailed physics models, the interactions of these physics at the interface between natural and engineered systems, and the impact these physics have on the optimized design, control, and operations of carbon transport systems at continental scales. The proposed solutions will be implemented as a new, open source modeling software that reflects the effects of physics in engineering economics.

Technical Outcomes

To the best of this team's knowledge, this project has yielded the first mathematical model of carbon dioxide transport in pipelines that is amenable to optimization formulations. The project has shown that incorporating a model of pipeline physics and engineering constraints effects the choice of a least cost network design for carbon capture and sequestration-not including such features can yield results that underestimate the costs to meet carbon capture targets by as much as 10%.

Publications

Presentation Slides

Bent, R. W. Optimizing Carbon Capture & Sequestration Planning subject to Physics & Engineering Constraints. Presented at *UC-National Lab Fees Research Program Workshop*, Online, New Mexico, United States, 2021-05-06 - 2021-05-06. (LA-UR-21-24192)

Bent, R. W., K. Sundar, S. Srinivasan, B. Chen, A. V. Zlotnik, V. Gyrya and K. Terada. Modeling Compressible Fluid Transport At Scale For Carbon Dioxide Sequestration. Presented at *Informs Annual Meeting*, Anaheim, California, United States, 2021-10-24 - 2021-10-24. (LA-UR-21-29248)

Carbon Dioxide Conversion to Fuels and Chemical Feedstocks

Piotr Zelenay
20210800ER

Project Description

This research is focused on energy security and climate change, which are arguably two of the most pressing issues facing the United States (US). The ultimate project goal is to valorize carbon dioxide emissions from point-sources and direct air capture through cutting-edge science and novel carbon dioxide conversion electrocatalysts (for the electrochemical route) and catalysts (for the thermochemical route). The impact and importance of this project goes well beyond Department of Energy/National Nuclear Security Administration; in fact, its impact is global with respect to global warming. In terms of energy security, the ability to convert carbon dioxide (CO_2) to chemical feedstocks and renewable fuels (aviation, maritime, transportation) provides the ultimate in energy security by eliminating the need of traditional carbon sources such as fossil fuels or biomass.

Technical Outcomes

This project established a research & development base at Los Alamos for carbon dioxide (CO_2) conversion to value-added products via electrochemical and thermochemical routes. In electrochemical conversion route, we designed a new type of bimetallic catalysts and optimized their performance. In the thermochemical conversion route, we analyzed and developed the thermodynamics phase diagram of reactant and product mixtures, built a new continuous reactor for thermochemical CO_2 conversion, designed and synthesized a novel bifunctional heterogeneous catalyst.

Epitope mapping and crystal structures of neutralizing Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) antibodies

Julian Chen
20210949ER

Project Description

The coronavirus (COVID-19) pandemic has presented an unprecedented health challenge, and is a threat to the nation's economic and military interests. The rise of variants of the virus around the world emphasize the need for continued vigilance, through the development of new tools to treat severe cases of COVID-19, as well as enhanced methods of detecting the virus and its variants. We have isolated antibodies that can serve two purposes, as a means of early detection of the virus, and as treatments for severe cases of the illness. Our proposed work will bring these antibodies closer to being useful tools that can be used to combat this current pandemic, while preparing us for future ones.

Technical Outcomes

Two Los Alamos developed antibodies were chosen for their ability to neutralize the virus. The antigen-binding fragments of both antibodies were crystallized, as was a putative complex of the antibody and their target. Two complementary methods were deployed to map the binding regions (epitopes) on the SARS-CoV-2 spike protein receptor binding domain for the two antibodies.

Publications

Presentation Slides

Lillo, A. M. In vitro evolution-enabled selection of affinity reagents against bio/chem-threats. . (LA-UR-21-27539)

Perovskite Materials for Driving Carbon Dioxide Photo-Reduction

Rajinder Singh
20210950ER

Project Description

Increasing carbon dioxide (CO2) concentration in atmosphere due to utilization of hydrocarbon fuel sources (e.g. coal and natural gas) for power, energy and fuels production is significant energy security challenge. With increasing energy demand and slow paced transition to renewable energy sources, CO2 emissions reduction in an economically viable way on on large scale is a critical challenges. CO2 conversion to fuels using solar energy is a sustainable pathway to reduce CO2 emissions. However, CO2 is a very stable molecule, and tremendous energy is required to initiate CO2 reduction. The goal of this project is to leverage leading pervoskite-based solar cell materials for efficient use of abundant sunlight and water for CO2 conversion into valuable products. Pervoskite materials have unprecedented light conversion potential, and are currently transitioning to commercialization for solar power production. Using this emerging clean energy platform lays the foundation for an efficient CO2 recycling essential for a carbon neutral or negative economy.

Technical Outcomes

The reduction in the solar-light conversion efficiency of the perovskite materials in humid/carbon dioxide correlated well with relative humidity. The tolerance and light harvesting efficiency recovery of the perovskite solar cells under intermittent (ON/OFF) light in the presence of humid carbon dioxide environments was demonstrated. No measurable carbon dioxide reduction was observed which can be attributed to the reduced solar cell efficiency in humid carbon dioxide environments and/or low carbon dioxide sorption capacity.

Publications

Journal Articles

Wenson, G., H. V. Thakkar, H. Tsai, J. Stein, R. P. Singh and W. Nie. Mixed cation perovskite solar cells' degradation and recovery behaviors in carbon dioxide and moisture environment. Submitted to *ACS energy Letters*. (LA-UR-21-31873)

The ecology and evolution of Hantaviridae in the Americas

Ethan Romero-Severson
20210957ER

Project Description

Segmented viruses represent a danger to public health not only because they are deadly--Sin Nombre virus, a type of segmented hantavirus, has greater than 50% fatality--but also because their genomic segments can rearrange to form new viruses that have the potential to infect new hosts and to evade the immune system. This project aims to address a key knowledge and methods gap concerning the study of hantaviruses (a type of segmented virus) in the Americas by developing new methods for studying the frequency, location, and timing of genomic reassortment in this family of viruses. Understanding the "where" and "when" of genomic reassortment is the first step in understanding the risk of the emergence of new and deadly hantaviruses.

Technical Outcomes

The goals of this proposal evolved over the course of the project to adapt to a lack of sufficiently high quality, publicly available data. The team shifted gears to establish collaborations with University of New Mexico (UNM) to generate new hantavirus data from the UNM Museum of Southwestern Biology. Likewise, The team expanded the range of the project to include intracellular and immunological modeling for the development of a more comprehensive hantavirus research program.

Publications

Reports

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

Drug Discovery by Automated Adaptation of Chemical Structure and Identity

Christopher Neale
20200543ECR

Project Description

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

Publications

Journal Articles

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

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

Reports

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

Posters

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

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

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

Elena Giorgi
20200554ECR

Project Description

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

Publications

Journal Articles

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

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

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

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

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

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

Presentation Slides

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

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

Posters

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

Photochemistry of Actinides in Ionic Liquids for Advanced Separations

Janelle Droessler
20200561ECR

Project Description

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

Computational and Experimental Bioprospecting of Algae for Antimicrobial Compounds

Blake Hovde
20200562ECR

Project Description

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

Publications

Journal Articles

Kwon, T., B. Hovde and E. R. Hanschen. Addressing the scarcity of eukaryotic algal genome annotation: BUSCO application for gene prediction in 134 unannotated algal genomes. Submitted to *Cell Genomics*. (LA-UR-21-30119)

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

Posters

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

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

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

Chelsea Neil
20210640ECR

Project Description

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

Publications

Journal Articles

Jones, A. C., M. T. Pettes, A. Londono Calderon, S. Oglesby, S. A. Ivanov, D. Pete and S. Chabi. Manufacturing of Complex Si/C Structures: Exploring SixCy Materials. Submitted to *Nanotechnology*. (LA-UR-22-21434)

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

Presentation Slides

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

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

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

Sandipkumar Maurya
20210680ECR

Project Description

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

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

Kane Bennett
20210686ECR

Project Description

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

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

Alexandra Jonko
20210689ECR

Project Description

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

Publications

Journal Articles

Zhai, L., D. R. Coyle, D. Li and A. Jonko. Fire, insect, and disease-caused tree mortalities increased in forests of greater structural diversity during drought. Submitted to *Journal of Ecology*. (LA-UR-21-28195)

Presentation Slides

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

Illuminating the Subsurface with Nonlinear Behavior

Andrew Delorey
20190552ECR

Project Description

The country's energy and environmental security depends on effective use of the subsurface because most of our energy comes from the subsurface and most of our waste material such as nuclear, brine (produced during oil and gas extraction) and CO_2, is or will be stored in the subsurface. Despite this importance, we have very little timely information on subsurface conditions that affect the performance of these systems while avoiding hazards such as induced earthquakes and leakage of waste materials. Fractures at all scales are important to the performance of subsurface systems because they form the pathways for fluid migration and because their coalescence leads to earthquakes and containment failures. We are developing a new way to measure and monitor fractures in the subsurface using background seismic noise. As seismic waves travel through fractured materials, their travel times are perturbed by how weak or strong the contacts are across the fractures. Weak fracture contacts typically indicate that permeability is increasing and decreasing material strength, while stronger contacts typically indicate decreasing permeability and increasing material strength. These relationships have been observed in laboratory samples of rocks. Observing these relationships in the Earth will substantially contribute to our effective use of the subsurface.

Technical Outcomes

This project measured nonlinear behavior in the Earth at three sites, Parkfield, California, North Central Oklahoma, and North Central New Mexico. In Parkfield, key properties of elastic hysteresis were constrained. In Oklahoma and New Mexico, anisotropy was measured in nonlinear behavior related to the orientation of the principal stress orientations. Both sets of results are important links to theory and laboratory studies.

Publications

Journal Articles

Delorey, A. A. Estimation of the orientation of stress in the Earth's crust without earthquake or borehole data. 2021. *Communications Earth & Environment*. **2** (1): 190. (LA-UR-20-29378 DOI: 10.1038/s43247-021-00244-1)

. G. R. A. *. B. G. H. R. *. J. P. A. Delorey, A. A., A. A. Delorey, R. A. Guyer and P. A. Johnson. Probing the Damage Zone at Parkfield. 2021. *Geophysical Research Letters*. **48 (13): e2021GL093518. (LA-UR-20-28743 DOI: 10.1029/2021GL093518)

Presentation Slides

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

Delorey, A. A., G. Bokelmann, C. W. Johnson and P. A. Johnson. Measuring the orientation of SHmax using ambient seismic noise. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31959)

Molecular Multi-Actinide Cores to Model Surface Reactivity

Aaron Tondreau
20190570ECR

Project Description

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

Technical Outcomes

The monometallic caged metal model systems investigated were thoroughly successful. The expanded naphthyridine cage was synthesized and characterized and installation of lanthanide surrogates was attempted, but structural characterization was unsuccessful due to poor insolubility of the metal complexes. Further derivatization of naphthyridine cages proved incredibly difficult because the 'linkages' are difficult, and the final cage was incredibly sensitive to hydrolysis from adventitious water. Progress was made toward reduction and desired bimetallic caged complexes.

Publications

Journal Articles

Klamm, B. E., K. Bhardwaj, S. M. Greer, H. D. Root, S. Sharma, C. J. Windorff, M. M. MacInnes, S. H. Carpenter, T. E. Albrecht-Schonzart, B. L. Scott, B. Stein, S. A. Kozimor and A. Tondreau. Caging Plutonium. Submitted to *Inorganic Chemistry*. (LA-UR-21-28031)

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

Presentation Slides

Tondreau, A. and S. H. Carpenter. Generating ligand scaffolds for mixed f- and d-block heterobimetallic architectures. Presented at *ACS National Conference, Spring 2021*, Online, California, United States, 2021-04-05 - 2021-04-05. (LA-UR-21-23306)

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

Carrie Manore
20190581ECR

Project Description

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

Technical Outcomes

The project developed an accurate model of mosquito population dynamics, started ongoing collaborations with public health and mosquito control boards in Toronto, Washington state, and South Carolina to acquire data, cleaned that data (no small task for typical mosquito trap data), acquired satellite and weather and hydrology data for each of the data-intensive regions, and applied multiple models to the data with high accuracy in predicting mosquito trap counts.

Publications

Journal Articles

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

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

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

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

*Romero-Alvarez, D., N. Parikh, D. Osthus, K. Martinez, N. Generous, S. Del Valle and C. A. Manore. Google Health Trends performance reflecting dengue incidence for the Brazilian states. 2020. *BMC Infectious Diseases*. **20** (1): 252. (LA-UR-19-31066 DOI: 10.1186/s12879-020-04957-0)

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

Reports

Spencer, J. A., D. A. Shutt, S. K. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Working paper: epidemiological parameter review and comparative dynamics of influenza, respiratory syncytial virus, rhinovirus, human coronavirus, and adenovirus. Unpublished report. (LA-UR-20-21024)

Presentation Slides

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

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

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

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

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

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

Spencer, J. A., D. A. Shutt, S. K. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Preparing for the Next Pandemic: Distinguishing Parameters and Properties of Respiratory Viruses. Presented at *MIDAS Network Annual Meeting 2021*, Virtual, New Mexico, United States, 2021-05-10 - 2021-05-13. (LA-UR-21-24217)

Spencer, J. A., D. A. Shutt, S. K. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Preparing for the Next Pandemic: Distinguishing Parameters and Properties of Respiratory Viruses. Presented at *MIDAS Network Annual Meeting 2021*, Virtual, New Mexico, United States, 2021-05-10 - 2021-05-13. (LA-UR-21-24215)

Spencer, J. A., D. A. Shutt, S. K. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Preparing for the Next Pandemic: Distinguishing Parameters and Properties of Respiratory Viruses. Presented at *Midas Network Annual Meeting 2021*, Virtual, New Mexico, United States, 2021-05-10 - 2021-05-13. (LA-UR-21-24216)

Posters

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

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

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

Other

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

Investigating Actinide-Based Molecular Magnetism with Electron Paramagnetic Resonance

Benjamin Stein
20180759PRD4

Project Description

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

Publications

Journal Articles

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

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

Posters

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

Multiscale Quantitative Description of Drug Resistance Mechanisms in Bacterial Systems

Sandrasegaram Gnanakaran
20190644PRD3

Project Description

This project builds foundational capability for designing next-generation antibacterial drugs; with a focus on countermeasure development for treating pathogen infection; the understanding gained in this project will have broad applications in biosecurity. At present, we rely on antibiotics for the treatment of bacterial infections encountered in public health and bio-threat scenarios; however, the rapid emergence of antibiotic resistance poses a major hurdle to effective treatment. Our inability to design novel drugs for antibiotic applications is in part due to a lack of understanding of the mechanisms of multi-drug resistance. This project will provide systems-level understanding of the operating principles governing how antibiotics are transported out of bacterial membranes by efflux pumps, dominant mechanism of drug resistance in many potential select-agent pathogens. The combined approach of multi-scale mathematical models and big data from large-scale simulations and high-throughput experiments proposed in this project is not limited to biological system, but rather can be applied to understand other multi-scale problems of interest to the Department of Energy(DOE)/ National Nuclear Security Administration(NNSA). It has the potential to connect the statistical physics based multi-scale models to high performance computing help solidify DOE's exascale computing initiatives, thereby strengthening the key NNSA goal of stockpile stewardship.

Publications

Journal Articles

Manrique Charry, P. D., S. El Oud and N. Johnson. A Generalized Gelation Theory and the Growth of Online Extreme Communities. Submitted to *Nature Physics*. (LA-UR-20-25198)

Manrique Charry, P. D. and S. Gnanakaran. Microscopic Approach to Intrinsic Antibiotic Resistance. Submitted to *Nature Physics*. (LA-UR-20-27348)

Johnson, N., N. Velasquez, O. Jha, H. Niyazi, R. Leahy, N. Johnson Restrepo, R. Sear, P. D. Manrique Charry, Y. Lupu, P. Devkota, S. Wuchty and B. Goldberg. Covid-19 infodemic reveals new tipping point epidemiology and a revised R formula. Submitted to *Nature Human Behaviour*. (LA-UR-20-25193)

Velasquez, N., P. D. Manrique Charry, R. Sear, R. Leahy, N. Johnson Restrepo, L. Illary, Y. Lupu and N. Johnson. Hidden order across online extremist movements can be disrupted by nudging collective chemistry. Submitted to *Scientific Reports*. (LA-UR-21-21269)

Posters

Manrique Charry, P. D., R. Henderson, S. Chakraborty, T. K. Nguyen, R. Mansbach, K. Wiehe, B. T. M. Korber and S. Gnanakaran. USING GRAPHS TO ANALYZE SARS-COV-2 MUTATIONS. Presented at *Biophysics Society Annual Meeting*, Boston, Massachusetts, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-21108)

Manrique Charry, P. D. and S. Gnanakaran. Multi-scale Antimicrobial Resistance Approach Featuring Cell-to-cell Heterogeneity Reveals Tradeoff Between Optimal Fitness and Colony Survival. Presented at *World Microbe Forum*, Virtual, New Mexico, United States, 2021-06-20 - 2021-06-24. (LA-UR-21-25653)

Toward a Universal Description for Aqueous Solutions

Alp Findikoglu
20190653PRD4

Project Description

Meeting humanity's growing demand for fresh water is a major challenge. In particular, affordable methods to desalinate Earth's vast saline water resources remain elusive. One promising approach to meeting this challenge is supercritical water desalination, which is based on using high temperatures and pressures to manipulate water's properties and hence its ability to precipitate salts. Supercritical desalination is very well-suited for integration into other industrial processes; however, a number of both fundamental and practical issues exist. The proposed work combines both theoretical and experimental studies to make significant advances in our understanding of how salt ions and water behave in supercritical water. The knowledge generated by this work should have direct relevance for the development of the supercritical water desalination processes.

Publications

Journal Articles

*Yoon, T. J., L. A. Patel, T. Ju, M. J. Vigil, A. T. Findikoglu, R. P. Currier and K. A. Maerzke. Thermodynamics, dynamics, and structure of supercritical water at extreme conditions. 2020. *Physical Chemistry Chemical Physics*. **22** (28): 16051-16062. (LA-UR-20-22874 DOI: 10.1039/D0CP02288H)

Yoon, T., E. P. Craddock, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Electrical Conductances and association constants in dilute aqueous NdCl 3 solutions from 298 to 523 K along an isobar of 25 MPa. Submitted to *Journal of Chemical & Engineering Data*. (LA-UR-21-30907)

Yoon, T., E. Y. Raby, P. Sharan, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. Electrical characterization of binary mixtures and ternary nanostructured fluids composed of water, 2-propanol, and n-hexane. Submitted to *Journal of Molecular Liquids*. (LA-UR-20-30449)

Yoon, T., J. D. Riglin, P. Sharan, R. P. Currier, K. A. Maerzke and A. T. Findikoglu. An in-situ conductometric apparatus for physicochemical characterization of solutions and in-line monitoring of separation processes at elevated temperatures and pressures. Submitted to *Measurement Science & Technology*. (LA-UR-21-29440)

Yoon, T., K. A. Maerzke, R. P. Currier and A. T. Findikoglu. PyOECP: A flexible open-source software library for estimating and modeling the complex permittivity based on the open-ended coaxial probe (OECP) technique. Submitted to *Computer Physics Communications*. (LA-UR-21-29438)

*Yoon, T., M. J. Vigil, E. Y. Raby, R. P. Singh, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Dielectric relaxation of neodymium chloride in water and in methanol. 2020. *Journal of Molecular Liquids*. **308**: 112981. (LA-UR-19-32739 DOI: 10.1016/j.molliq.2020.112981)

Presentation Slides

Yoon, T., L. A. Patel, M. J. Vigil, A. T. Findikoglu, K. A. Maerzke and R. P. Currier. Understanding the Specific Conductance of NaCl Solutions in Water at Elevated Temperatures and Pressures. Presented at *2020 Virtual AIChE Annaul Meeting*, Los Alamos, New Mexico, United States, 2020-11-16 - 2020-11-20. (LA-UR-20-28738)

Forecasting Valley Fever Disease Risk Using Machine Learning

Carrie Manore
20200682PRD1

Project Description

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

Publications

Journal Articles

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

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

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

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

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

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

Tong, D., M. E. Gorris, K. Ardon-Dryer, T. Gill, J. Wang and L. Ren. Comments on "No Consistent Link Between Dust Storms and Valley Fever (Coccidioidomycosis)". Submitted to *GeoHealth*. (LA-UR-22-22270)

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

Presentation Slides

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

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

Gorris, M. E., J. Neumann, P. Kinney, M. Sheahan and M. Sarofim. Economic valuation of Valley fever (coccidioidomycosis) in response to climate change. Presented at *American Geophysical Union Fall Meeting*

2021, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31689)

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

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

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

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

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

Other

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

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

Charles Abolt
20200771PRD4

Project Description

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

Publications

Journal Articles

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

Presentation Slides

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

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

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

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

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

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

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

Posters

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

Other

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

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

Identifying Geometric Constraints Imposed by Antibiotics on Biomolecular Machines

Karissa Sanbonmatsu
20210759PRD1

Project Description

The project outlined here focusses on the development of novel antibiotics for battling the looming threat of antimicrobial resistant pathogens. The current coronavirus (COVID-19) pandemic has shown how susceptible the global community is to a pandemic level threat. Resistant pathogens represent another pandemic level threat and with the lack of commercial interest in novel antibiotics it is critical that the public sector invest in their development. Development of novel antibiotics to combat pandemic level threats addresses the missions of biothreat as well as Pathogen Detection and Countermeasures. As resistant pathogens are becoming more common due to overuse and over prescription of antibiotics it is likely that they can be engineered. Using integrative electron microscopy and simulations approaches we aim to not only understand how conventional antibiotics work but provide a platform for the development and initial screening of novel antibiotics. This will help provide operational countermeasures against looming pathogenic threats.

Valorization of Lignin for the Production of High Performance Sustainable Aviation Fuels

Cameron Moore
20210762PRD1

Project Description

This project proposes to develop a scalable process for converting lignin from biomass into high performance aviation fuel. The project will include development of new chemistry as well as fuel testing to determine the suitability of the resulting products for aviation applications. This work will provide a basis for capturing the potential value of lignin which is often discarded or combusted. Valorization of lignin offers one potential route to enabling cost-competitive biofuels to enter the market and move the aviation industry toward their goal of reducing carbon dioxide (CO_2) emissions by 2050. In addition, this work will help strengthen the nation's energy security by developing domestic production pathways for aviation fuel using agricultural waste products as feedstocks.

Pore Size and Wettability of Control Electrodes for Next Generation Hydrogen Fuel Cells

Rangachary Mukundan
20210915PRD2

Project Description

This study will demonstrate a powerful platform to better understand water transport in Polymer electrolyte membrane fuel cells (PEMFC) by developing a method for introducing controlled pore sizes into an electrode and tuning their wettability. Extensive characterization of the electrode structure and its performance as a fuel cell cathode will provide insights into the role of water management in increasing the utilization of platinum catalyst within the electrode. This project is expected to lead to design rules for the next generation of electrode that are not just random mixtures of porosity, catalyst, and ionic and electronic conducting phases. Since, the Platinum catalyst used in the electrode is the largest contributor (up to 53%) to the high cost of PEMFC systems, improved utilization of the catalyst can dramatically improve power density and decrease material costs. The results of this project will be applicable to other energy conversion devices like water and carbon dioxide (CO_2), electrolyzers, and in desalination and hydrogen pumping applications.

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

Matthew Hoffman
20210952PRD3

Project Description

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

Publications

Journal Articles

Coulson, S. L., M. Lubeck, J. X. Mitrovica, E. Powell, J. L. Davis and M. J. Hoggard. The Global Fingerprint of Modern Ice-Mass Loss on 3-D Crustal Motion. Submitted to *Geophysical Research Letters*. (LA-UR-21-27647)

Presentation Slides

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

Molecular Basis of Ras-related Cancers

Angel Garcia
20170692PRD4

Project Description

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

Technical Outcomes

The atomistic simulations explored the dynamics of proteins in the milliseconds time scale, 10-100 longer than most simulations of KRAS4b (Kirsten rat sarcoma viral oncogene homolog 4b) previously recorded. The project developed and used large scale, lower resolution, models to study the dynamics that occur in time scales not accessible to atomistic simulations. The energy landscape of KRas4B monomers and dimers, bound to lipid bilayers was revealed.

Publications

Journal Articles

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

Ngo, A. V., S. Sarkar, C. A. Neale and A. E. Garcia. How Anionic Lipids Affect the Spatiotemporal Properties of KRAS4B on Model Membranes in Millisecond All-atom Molecular Dynamics Simulations. Submitted to *Biophysical Journal*. (LA-UR-20-21331)

Ngo, V. A. and R. K. Jha. Identifying key determinants and dynamics of SARS-CoV-2/ACE2 tight interaction. 2021. *PLOS ONE*. **16** (9): 0259705. (LA-UR-20-24876 DOI: 10.1371/journal.pone.0257905)

*Wang, Y., R. K. Finol-Urdaneta, A. N. Van, R. J. French and S. Y. Noskov. Bases of Bacterial Sodium Channel Selectivity Among Organic Cations. 2019. *Scientific Reports*. **9** (1): 15260. (LA-UR-19-29893 DOI: 10.1038/s41598-019-51605-y)

Unusual Oxidation States and Covalency-Tuning in Transuranic Molecules

Conrad Goodwin
20180703PRD1

Project Description

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

Technical Outcomes

A suite of lanthanide, uranium, and transuranium molecules were isolated and characterized with the proposed phosphole and other chelates, a body of work that significantly advanced comprehension of f-element electronic structure and bonding. High visibility signature results include the first quantification of californium-carbon bonding, neptunium carbon double bonds, and americium-selenium bonds. The postdoctoral researcher this project supported has contributed to over 10 publications (with more in preparation) from his efforts on this project.

Publications

Journal Articles

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

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

Dutkiewicz, M. S., C. A. P. Goodwin, M. Perfetti, A. J. Gaunt, J. Griveau, E. Colineau, A. Kovacs, A. J. Wooles, R. Caciuffo, O. Walter and S. T. Liddle. A Terminal Neptunium(V)-Mono(Oxo) Complex. Submitted to *Nature Chemistry*. (LA-UR-21-27198)

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

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

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

P. Goodwin, C. A., A. W. Schlimgen, T. E. Albrecht-Sch\xc3\xb6nzart, E. R. Batista, A. J. Gaunt, M. T. Janicke, S. A. Kozimor, B. L. Scott, L. M. Stevens, F. D. J. White and P. Yang. Structural and Spectroscopic Comparison of Soft-Se vs. Hard-O Donor Bonding in Trivalent Americium/Neodymium Molecules. 2021. *Angewandte Chemie International Edition*. **60** (17): 9459-9466. (LA-UR-21-20831 DOI: 10.1002/anie.202017186)

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

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

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

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

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

P. Goodwin, C. A., M. T. Janicke, B. L. Scott and A. J. Gaunt. [AnI3(THF)4] (An = Np, Pu) preparation bypassing An0 metal precursors: access to foundational Np3+/Pu3+ nonaqueous and organometallic complexes. Submitted to *Journal of the American Chemical Society*. (LA-UR-21-27540)

P. Goodwin, C. A., S. R. Ciccone, S. Bekoe, S. Majumdar, B. L. Scott, J. W. Ziller, A. J. Gaunt, F. Furche and W. J. Evans. 2.2.2-Cryptand Complexes of Neptunium(III) and Plutonium(III). Submitted to *Angewandte Chemie - International Edition*. (LA-UR-21-27533)

*Greer, S. M., \. \xc3\x9cngor, R. J. Beattie, J. L. Kiplinger, B. L. Scott, B. W. Stein and C. A. P. Goodwin. Low-spin 1,1#-diphosphametallocenates of chromium and iron. 2021. *Chemical Communications*. **57** (5): 595-598. (LA-UR-20-20981 DOI: 10.1039/D0CC06518H)

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

Su, J., T. Chesisson, A. McSkimming, C. A. P. Goodwin, I. M. DiMucci, T. Albrecht-Schonzart, B. L. Scott, E. R. Batista, A. J. Gaunt, S. A. Kozimor, P. Yang and E. J. Schelter. Complexation and Redox Chemistry of Neptunium, Plutonium and Americium with a Hydroxylaminato Ligand. Submitted to *Chemical Science*. (LA-UR-21-27074)

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

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

Reports

P. Goodwin, C. A., A. J. Gaunt, M. T. Janicke, N. Kaltsoyannis and B. L. Scott. A comparison of metal-carbon bonding in 4f and 5f metallocene N-heterocyclic carbene complexes. Unpublished report. (LA-UR-21-26428)

P. Goodwin, C. A., A. J. Gaunt, M. T. Janicke and B. L. Scott. Results to share with University of Manchester collaborator. Unpublished report. (LA-UR-21-23305)

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

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

Presentation Slides

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

P. Goodwin, C. A. assorted non-transuranium, d-block, main-group structures, pictures. . (LA-UR-21-27222)

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

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

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

P. Goodwin, C. A., S. M. Greer, B. Stein and A. J. Gaunt. LANL – UoM collaboration with S. T. Liddle. . (LA-UR-21-23256)

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

P. Goodwin, C. A. and A. J. Gaunt. Cyclic voltammetry (C124) on [Np{N(C2H4NSiiPr3)3}] – [Np(TrenTIPS)] a Np(III) coordination complex. . (LA-UR-21-26648)

P. Goodwin, C. A. and A. J. Gaunt. f-element methanide and methanediide complexes. . (LA-UR-21-27191)

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

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

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

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

Posters

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

New First Row Transition Metal Based Catalysts for Sustainable Energy Production

John Gordon
20180705PRD1

Project Description

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

Technical Outcomes

This work resulted in a series of new catalytic transformations related to the upgrading of bio-sourced molecules into useful chemicals. Particularly noteworthy, is that a number of the systems uncovered in this project have been able to address technical challenges associated with the need to promote desired chemical transformations selectively and with high efficiency.

Publications

Journal Articles

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

*Batrice, R. J. and J. C. Gordon. Powering the next industrial revolution: transitioning from nonrenewable energy to solar fuels via CO2 reduction. *RSC Advances*. (LA-UR-20-26316 DOI: 10.1039/D0RA07790A)

Reports

Gordon, J. C. New First Row Metal Based Catalysts for Sustainable Energy Production. Unpublished report. (LA-UR-21-28867)

Presentation Slides

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

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

Ivan Popov
20180710PRD1

Project Description

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

Technical Outcomes

This project developed theoretical principles needed to develop charge carriers with higher energy density characteristics that could carry >2 electrons per molecule. The team showed it is possible to achieve cell potentials of >3 volts by stabilizing metals in a wide range of oxidation states with the help of specific ligands. Further modification of the ligands with various electron donating group (EDG) and electron withdrawing group (EWG) substituents can help achieve even higher cell potentials.

Publications

Journal Articles

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

. P. I. A. *. H. C. R. *. G. T. S. *. Z. P. R. *. M. L. M. *. S. K. F. *. B. C. H. *. A. R. J. *. B. E. R. *. Y. P. *. S. J. C. Bessen, N. P., I. A. Popov, E. R. Batista and P. Yang. Complexation of Lanthanides and Heavy Actinides with Aqueous Sulfur-Donating Ligands. 2021. *Inorganic Chemistry*. **60 (9): 6125-6134. (LA-UR-20-27724 DOI: 10.1021/acs.inorgchem.1c00257)

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

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

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

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

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

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

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

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

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

*Rice, N. T., I. A. Popov, D. R. Russo, T. P. Gompa, A. Ramanathan, J. Bacsa, E. R. Batista, P. Yang and H. S. La

Pierre. Comparison of tetravalent cerium and terbium ions in a conserved, homoleptic imidophosphorane ligand field. 2020. *Chemical Science*. **11** (24): 6149-6159. (LA-UR-20-22218 DOI: 10.1039/D0SC01414A)

*Sharma, S., G. A. Andrade, S. Maurya, I. A. Popov, E. R. Batista, B. L. Davis, R. Mukundan, N. C. Smythe, A. M. Tondreau, P. Yang and J. C. Gordon. Iron-iminopyridine complexes as charge carriers for non-aqueous redox flow battery applications. 2021. *Energy Storage Materials*. **37**: 576-586. (LA-UR-20-28348 DOI: 10.1016/j.ensm.2021.01.035)

Tkachenko, N. V., I. A. Popov, A. Mu\xc3\xb1oz-Castro, Z. M. Sun and A. I. Boldyrev. Bridging Aromatic/Antiaromatic Units: Recent Advances in Aromaticity and Antiaromaticity in Main-group and Transition-Metal Clusters from Bonding and Magnetic Analyses. 2021. *European Journal of Inorganic Chemistry*. ejic.202100519. (LA-UR-20-27965 DOI: 10.1002/ejic.202100519)

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

T. N. V. *. P. I. A. *. Q. L. *. M. A. *. B. A. I. *. S. Z. Xu, Y. *. and I. A. Popov. Ternary aromatic and anti-aromatic clusters derived from the hypho species [Sn2Sb5]3–. 2021. *Nature Communications*. **12** (1): 4465. (LA-UR-20-28353 DOI: 10.1038/s41467-021-24706-4)

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

Presentation Slides

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

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

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

Posters

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

Other

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

Enabling Artificial Selection Programs through Characterizing the Lifecycle of Green Algae

Shawn Starkenburg
20190616PRD1

Project Description

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

Technical Outcomes

Characterizing the life cycle of Scenedesmus obliquus ran into several unexpected challenges and despite novel approaches, including isolating new Scenedesmus strains and temperature and nutrient shock deprivation experiments, reproduction was not achieved. Therefore, a meta-analysis on algae genomics was performed, which is related due to application of genomics in both projects. The team found a problematic decline in the quality of recent algal genomics projects and provide recommendations to the field address these shortcomings.

Publications

Journal Articles

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

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

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

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

Reports

Hanschen, E. R. Enabling Artificial Selection Programs through Characterizing the Lifecycle of Green Algae. Unpublished report. (LA-UR-21-24146)

Presentation Slides

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

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

Posters

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

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

Geochemical-Geomechanical Feedback in Stressed Fracture Systems

James Carey
20200769PRD3

Project Description

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

Technical Outcomes

The project expanded the capabilities of a unique Los Alamos facility that allows direct x-ray imaging of dynamic rock fracturing to image fluid-rock reactions that result in mineral precipitation. The results show the highly localized nature of precipitation reactions that restricts fluid transport despite relatively small volumes of reaction product. While the postdoctoral fellow departed early for a tenure track position at Penn State, this work will continue through a now-established collaboration.

Agile System for Electrochemical Dissolution of Bulk Actinide Oxides

Benjamin Karmiol
20210556MFR

Project Description

Many actinide oxide bearing materials exist in the Department of Energy (DOE) complex. These materials often need to be stabilized for disposal or recovered for reuse. This can be achieved by burning the materials or dissolving and purifying the materials. Burning introduces certain risks (high energy, chemical reactions), and currently the only way to dissolve these materials is to use a boiling nitric acid fluoride ion solution which poses a high safety risk. The proposed research will develop a versatile electrochemical system that uses various catalysts to dissolve refractory actinide oxides, such as those described above. The system would allow for continuous reuse of the solution through electrolytic regeneration of the catalyst, elimination of fluoride ion, and dissolution at ambient temperatures. Testing will include determining rates of Plutonium Dioxide (PuO2) dissolution using various catalysts. Information from these studies will allow for the design of a bulk actinide oxide dissolution systems that could be tailored (quantities of feed, types of feed, end-use of product, etc.) for low cost to meet dissolution needs. This project aims to develop customized actinide oxide dissolution options that could be deployed quickly, extending the capabilities of the Los Alamos Plutonium Facility (PF4).

Publications

Presentation Slides

Karmiol, B., J. E. Droessler and S. P. Walsh. Agile System for Electrochemical Dissolution of Bulk Actinide Oxides (L-MODS). Presented at *LANL Weapon's Capability Review*, Los Alamos, New Mexico, United States, 2021-08-23 - 2021-08-26. (LA-UR-21-28202)

Computational Modeling Tool for Rapid Performance Characterization of Novel High-explosive Design Geometries

Von Whitley
20210585MFR

Project Description

Research into high explosives (HEs) has produced a number of innovations the past few years. New explosives molecules, newer and less sensitive formulations have been developed, and newer and faster manufacturing methods have been developed. All of the innovations need to be computationally evaluated to determine if they are acceptable for use in non-special nuclear material (SNM) nuclear explosive applications. The sheer number of innovations that need to be evaluated has overwhelmed the computational resources available. Thus adoption of these newer innovations is currently hindered by the computational time that is needed to evaluate the changes. This research proposed to produce a computational design tool that substantially speeds up the computational efficiency needed to evaluate new experimental designs. With these speed increases, we will be able to do initial design assessments using a single central processing unit (CPU) instead of thousands of nodes on a supercomputer. Other design studies that were impossible because they required more CPUs than the supercomputers currently contain, e.g., full 3-Dimensional design studies, will now be possible using our current supercomputers. Obtaining results in a matter of seconds on a personal computer will dramatically reduce the cost and time required in the design of HE components.

Publications

Journal Articles

Lozano, E. and T. D. Aslam. Topological skeletons and local size of multidimensional objects using the fast sweeping method. Submitted to *Computers & Graphics*. (LA-UR-21-24854)

Posters

Whitley, V. H. and C. A. DeBurgomaster. Select Hugoniot Curves and Materials Data. . (LA-UR-21-30934)

Biotechnology for Regional Climate Resilience

Babetta Marrone
20210921DI

Project Description

With a changing climate comes risks associated with extreme heat, fire, drought, floods, hurricanes, and other climate and weather-related events. This project aims to develop tools and technologies to meet local to regional climate resilience and mitigation objectives with a focus on military applications: stationary bases; forward operating bases; and Humanitarian Assistance and Disaster Relief operations. Our aim is to develop tools and technologies to promote the use of waste carbon, including carbon dioxide, food waste, and plastics, to improve the environmental sustainability of military operations during climate and weather-related disasters. Our first goal is to create a new climate action geospatial tool that can be used to predict local- to country-scale potential for waste carbon development into desirable products (e.g. energy, water, biomaterials, fuel). Our second goal is to develop a biomanufacturing technology to convert waste carbon to usable products (building and construction materials, fuels). Our project will lay the groundwork to develop sustainable, biological solutions to critical needs for energy and materials in fixed or mobile military operations that enable adaptation and agility in response to challenges of climate change and extreme weather events.

Publications

Presentation Slides

Hernandez, M. M., A. D. Atencio, C. R. Gonzalez Esquer, B. L. Marrone and J. H. Dumont. Algae and Concrete Composites: Structural Materials as a CO_2 sink. Presented at *ACS Fall 2021 Meeting*, Boston, Massachusetts, United States, 2021-11-29 - 2021-12-02. (LA-UR-21-31590)

Data Driven Accelerated Fuel Qualification for Nuclear Fuels

Tammie Nelson
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Project Description

Nuclear power in the United States is provided by 96 commercial Light Water Reactors (LWRs). Economic improvement for the existing LWR fleet is pursued by extending the burn-up limits of the current fuel, for example, and developing new or refined fuel concepts. There is also significant interest in developing advanced reactors that could utilize non-Uranium Dioxide (UO2) fuel concepts. For burn-up extensions or new LWR fuels and advanced reactor fuels to be successfully deployed, the fuel must be qualified as safe by the regulator. For this to be economical, the process should be fast and predictable. However, in reality, fuel development is a lengthy process that relies heavily on full-scale, complex fuel tests that can take up to 25 years to complete. This is a serious hurdle that must be addressed. We intend to decrease this gap through the introduction of modern data science powered by machine learning (ML) into the existing modeling approach. This will ultimately enable accelerated fuel qualification (AFQ) by reducing the integral experiments needed for qualification. The approach will be demonstrated for uranium carbide and nitride (U(C,N)) fuels, which are of interest for several advanced reactor types and even as a UO2 replacement in LWRs.

Technical Outcomes

The project produced new physical insights into gas diffusion in nuclear fuel and set the stage for future developments in breakaway swelling models. The developed dislocation tracking shows great promise to describe damage accumulation in fuel. New physics for diffusion of vacancies, interstitials, and Xenon has been introduced to the cluster dynamics model. The team has shown that machine learning significantly increases predictive accuracy of fuel properties with substantially reduced computational cost.

Publications

Journal Articles

Kocevski, V., M. W. D. Cooper, A. Claisse and A. D. R. Andersson. Development and application of a uranium mononitride (UN) potential: thermomechanical properties and Xe diffusion. 2022. *Journal of Nuclear Materials*. 153553. (LA-UR-21-28424 DOI: 10.1016/j.jnucmat.2022.153553)

Reports

Nelson, T. R. Data Driven Accelerated Fuel Qualification for Nuclear Fuels. Unpublished report. (LA-UR-21-29429)

Presentation Slides

Craven, G. T. Machine learning approaches for thermodynamic and transport properties of fluids and materials. Presented at *Los Alamos - Arizona Days Conference 2021*, Los Alamos, New Mexico, United States, 2021-05-17 - 2021-05-18. (LA-UR-21-24657)

Kocevski, V., M. W. D. Cooper, A. Claisse and A. D. R. Andersson. Development and application of a UN potential to defect properties and high temperature elastic constants. Presented at *MiNES 2021*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-11. (LA-UR-22-20359)

Global Trends, Resiliency, and Recovery

Sara Del Valle
20210766DI

Project Description

The Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) pandemic and economic crisis is likely to push millions of people into extreme poverty, lead to food insecurity, and increase the risk of political and socioeconomic instability around the globe. These conditions coupled with environmental degradation, climate change, globalization, conflict, and future pandemics will lead to greater destabilization that threatens human existence. Thus, by systematically comparing four different regions around the globe (i.e., the United States, Brazil, India, and Sweden), we will characterize drivers leading to resiliency or lack thereof, post SARS-CoV-2, and predict potential recovery. This project aligns the Nation's and Laboratory's strategic initiatives and executive directives in understanding resiliency from global catastrophic events and help prepare the Nation for future disruptive events.

Technical Outcomes

The project was successful in achieving the following outcomes: 1) collecting, cleaning, and harmonizing heterogeneous data for six countries; 2) characterizing pandemic resilience using a data-driven approach; 3) characterizing economic recovery using input/output econometric models; and 4) comparing results against previously published studies and demonstrating enhancements over them.

Publications

Journal Articles

Barnard, M. J., R. Iyer, S. Y. Del Valle and A. R. Daughton. Impact of COVID-19 Policies and Misinformation on Social Unrest. Submitted to *PLOS One*. (LA-UR-21-29745)

VanDervort, L. J., P. Patelli, J. P. Schwenk, K. M. Martinez, T. R. Pitts, M. J. Barnard, K. A. Kaufeld, B. H. Mcmahon and S. Y. Del Valle. Multi-dimensional resilience: a quantitative exploration of disease outcomes and economic, political, and social resilience to the COVID-19 pandemic in six countries. Submitted to *PLOS One*. (LA-UR-21-31106)

Presentation Slides

Del Valle, S. Y. Real-Time Data Fusion to Guide Disease Modeling & Forecasting. Presented at *CNES Capability Review*, Los Alamos, New Mexico, United States, 2021-05-05 - 2021-05-07. (LA-UR-21-23452)

Del Valle, S. Y. Modeling COVID-19 with Agent-based Simulations: Challenges & Opportunities. Presented at *SAMSI:Pros and Cons of ABMs for Epidemic Modeling-Virtual Workshop*, Durham, North Carolina, United States, 2021-06-22 - 2021-06-22. (LA-UR-21-25833)

Mechanistic Studies of Human Disease

Nicolas Hengartner
20200002CR-CNL

Project Description

This project aims at modeling biological systems using computational and mathematical methods. Biological systems are modeled at different scales: atomistic (proteins, nuclei acids in various environments), systems of proteins described as members of an interacting (biochemical network), and dynamical non-linear systems that can show interesting behaviors in response to small perturbations. These models are used to model diseases and, potentially, to design new drugs that target specific proteins. The research is done in interdisciplinary teams that include biologists, physicists, and mathematicians. Postdoctoral fellows conduct the research under the supervision of Laboratory staff scientists. The modeling of signaling pathways related to cancer align with the Department of Energy's interest in developing high-performance computing and modeling approaches to help diagnose cancer patients. The development of new computational and modeling capability to study biomembranes will be relevant to health and biotechnology applications.

Publications

Journal Articles

*Berndsen, Z. T., S. Chakraborty, X. Wang, C. A. Cottrell, J. L. Torres, J. K. Diedrich, C. A. L\xc3\xb3pez, J. R. Yates, M. J. van Gils, J. C. Paulson, S. Gnanakaran and A. B. Ward. Visualization of the HIV-1 Env glycan shield across scales. 2020. *Proceedings of the National Academy of Sciences*. **117** (45): 28014-28025. (LA-UR-19-30964 DOI: 10.1073/pnas.2000260117)

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

Chakraborty, S., Z. T. Berndsen, N. W. Hengartner, B. T. M. Korber, A. B. Ward and S. Gnanakaran. Quantification of the Resilience and Vulnerability of HIV-1 Native Glycan Shield at Atomistic Detail. Submitted to *iScience (Cell Press)*. (LA-UR-19-30981)

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

Fox, Z. R. Extracting Trajectories from Stochastic Trajectories of Gene Expression. Submitted to *Physical Review Letters*. (LA-UR-22-21680)

Fox, Z. R., E. Barkai and D. Krapf. Aging power spectrum of membrane protein transport and other subordinated random walks. 2021. *Nature Communications*. **12** (1): 6162. (LA-UR-21-21176 DOI: 10.1038/s41467-021-26465-8)

Fox, Z. R., S. Fletcher, A. Fraisse, C. Aditya, S. Sosa-Carrillo, S. Gilles, F. Bertaux, J. Ruess and G. Batt. MicroMator: Open and Flexible Software for Reactive Microscopy. Submitted to *Nature Methods*. (LA-UR-21-22416)

Garcia, A. E., J. Janke, Y. Yu, V. Pomin, J. Zhao, C. Wang and R. Linhardt. Characterization of Heparin's Conformational Ensemble by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Spectroscopy. 2022. *Journal of Chemical Theory and Computation*. (LA-UR-20-28381 DOI: 10.1021/acs.jctc.1c00760)

Ke, R., S. Sanche, E. Romero-Severson and N. W. Hengartner. Fast spread of COVID-19 in Europe and the US and its implications: even modest public health goals require comprehensive intervention. Submitted to *Lancet Infectious Diseases*. (LA-UR-20-22635)

*Ke, R., S. Sanche, E. Romero-Severson and N. W. Hengartner. Estimating the reproductive number R0 of SARS-CoV-2 in the United States and eight European countries and implications for vaccination. 2021. *Journal of Theoretical Biology*. 110621. (LA-UR-20-25505 DOI: 10.1016/j.jtbi.2021.110621)

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

*Mansbach, R. A., T. Travers, S. Chakraborty and S. Gnanakaran. Graph-Directed Approach for Downselecting Toxins for Experimental Structure Determination. 2020. *Structure*. **18** (5): 256. (LA-UR-19-26210 DOI: 10.3390/md18050256)

Meyers, K., L. Liu, W. W. Lin, Y. Luo, M. T. Yin, Y. Wu, S. N. Wontakal, F. La Carpia, S. Fernando, M. Dowlatshahi, L. Joshua-Tor, J. Wolk, B. Alpert, M. Romney, B. K. Costabile, E. L. Gelardi, F. Vallese, O. B. Clarke, F. Mancia, A. Uhlemann, M. Sobiezczyk, A. S. Perelson, Y. Huang, E. A. Hod and D. D. Ho. Antibody Testing Documents the Silent Spread of SARS-CoV-2 in New York Prior to the First Reported Case. Submitted to *New England Journal of Medicine*. (LA-UR-20-23502)

Migliori, A. D. and C. A. Neale. RIT1 associates with a lipid bilayer via charge complementarity. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-19-32749)

*Neale, C. and A. E. Garcia. The Plasma Membrane as a Competitive Inhibitor and Positive Allosteric Modulator of KRas4B Signaling. 2020. *Biophysical Journal*. **118** (5): 1129-1141. (LA-UR-19-30243 DOI: 10.1016/j.bpj.2019.12.039)

Ngo, A. V., S. Sarkar, C. A. Neale and A. E. Garcia. How Anionic Lipids Affect the Spatiotemporal Properties of KRAS4B on Model Membranes in Millisecond All-atom Molecular Dynamics Simulations. Submitted to *Biophysical Journal*. (LA-UR-20-21331)

*C. S. *. M. R. A. *. K. B. *. G. S. Nguyen, K. *., S. Chakraborty, S. Gnanakaran, K. Nguyen and B. Korber. Exploring the Role of Glycans in the Interaction of SARS-CoV-2 RBD and Human Receptor ACE2. 2021. *Viruses*. **13** (5): 927. (LA-UR-21-22583 DOI: 10.3390/v13050927)

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

Pulavarti, S. V., J. B. Maguire, S. Yuen, J. S. Harrison, J. Griffin, P. Lakshamanane, E. A. Esposito, G. I. Makhatadze, A. E. Garcia, T. M. Weiss, E. H. Snell, B. Kuhlman and T. Szyperski. From Protein Design to the Energy Landscape of a Cold Unfolding Protein. Submitted to *Journal of the American Chemical Society*. (LA-UR-21-32367)

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

Rosenberger, D. G., J. S. Smith and A. E. Garcia. Modeling of peptides with classical and novel machine learning force fields: A comparison. Submitted to *Journal of Physical Chemistry B*. (LA-UR-20-27951)

Sarkar, S. Origin of concentration dependent reaction rates and their consequences. Submitted to *PNAS*. (LA-UR-20-24037)

Sarkar, S. and A. E. Garcia. Diffusive transport of biomolecules on compartmentalized membranes and its effect on reaction kinetics. Submitted to *Physical Review Letters*. (LA-UR-20-20267)

*Sarkar, S. and A. E. Garcia. Presence or Absence of Ras Dimerization Shows Distinct Kinetic Signature in Ras-Raf Interaction. 2020. *Biophysical Journal*. **118** (8): 1799-1810. (LA-UR-19-24762 DOI: 10.1016/j.bpj.2020.03.004)

Sarkar, S. and S. Choubey. Efficacy of information transmission in cellular communication. Submitted to *Physical Review Letters*. (LA-UR-20-28073)

Shirin, A., Y. T. Lin and F. Sorrentino. Data-driven Optimized Control of the COVID-19 Epidemics. Submitted to *Nature Communications*. (LA-UR-20-26630)

Smith, M. Z. and T. G. Schmitz. Spinning the Facts against Genetically Engineered Foods?. 2020. *Theoretical Economics Letters*. **10** (3): 458-480. (LA-UR-20-22385 DOI: 10.4236/tel.2020.103029)

Presentation Slides

Fox, Z. R. Computational design and control of stochastic gene expression in single cells. . (LA-UR-21-30734)

Kolade, B. A., J. C. Miner and R. F. Williams. Validating Experimental Results of toxins using Cheminformatics and Quantum Chemistry. Presented at *Student symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25834)

Migliori, A. D. Slides for FNLCR collaborators. . (LA-UR-19-32620)

Migliori, A. D., E. E. Wait, D. A. Armstrong and C. A. Neale. Computer-Guided Design of Medicines to Treat Cancer. . (LA-UR-20-22092)

Rosenberger, D. G. Using Kirkwood-Buff Integrals to estimate diffusion in mixtures.. . (LA-UR-20-28325)

Rosenberger, D. G. Collagen rigidity.. . (LA-UR-21-21244)

Rosenberger, D. G. A scientific journey from a mid-sized German city to the mountains of northern New Mexico.. . (LA-UR-21-21972)

Sarkar, S. Spatiotemporal organization of cell signaling. . (LA-UR-20-30389)

Sarkar, S. Emergent behaviors of cellular systems. . (LA-UR-21-25889)

Posters

Fox, Z. R., J. Ruess, G. Batt and Y. T. Lin. Fisher Information for Stochastic Gene Expression Trajectories and Cellular Timing Distributions. Presented at *Gordon Conference on Stochastic Physics in Biology*, Ventura, California, United States, 2021-10-17 - 2021-10-15. (LA-UR-21-29880)

Patel, L. A., C. A. Neale, T. J. Waybright and A. G. Stephen. GAP Positions Catalytic H-Ras Residue Q61 for GTP Hydrolysis in Simulations. Presented at *Ras Symposium*, Frederick,

Maryland, United States, 2021-05-24 - 2021-05-26. (LA-UR-21-24328)

The Dynamics of Systems Far From Equilibrium

Angel Garcia
20190496CR-CNL

Project Description

This project addresses the dynamics of fluid and metal systems out of equilibrium. The results are relevant for applications in carbon sequestration, ocean dynamics, and mixing of turbulent flows. At the most fundamental level, we will investigate computationally a range of fluid instabilities including low-Reynolds number porous media flows, multiphase compressible flows, and material interfaces in turbulent flows . Hydrodynamic instability, turbulence, and mixing have application in ocean and atmospheric modeling and in nuclear weapons physics.

Technical Outcomes

This project developed state of art the tools and applied these to perform outstanding science. Examples of this science include the execution of the first three-dimensional general relativistic, full transport neutrino radiation magnetohydrodynamics simulations of the black hole-accretion disk-wind system produced by the GW170817 merger; quantified the impacts of a Beaufort Gyre freshwater release, and established Multimessenger constraints on the neutron-star equation of state, among others. The project met all the goals of the proposal.

Publications

Journal Articles

Borovsky, J. E., G. L. Delzanno and K. Yakymenko. Pitch-Angle Diffusion in the Earth's Magnetosphere Organized by the Mozer-Transformed Coordinate System. Submitted to *Frontiers Astronomy and Space Sciences*. (LA-UR-21-31107)

*Brady, E., S. Stevenson, D. Bailey, Z. Liu, D. Noone, J. Nusbaumer, B. L. Otto-Bliesner, C. Tabor, R. Tomas, T. Wong, J. Zhang and J. Zhu. The Connected Isotopic Water Cycle in the Community Earth System Model Version 1. 2019. *Journal of Advances in Modeling Earth Systems*. **11** (8): 2547-2566. (LA-UR-19-28472 DOI: 10.1029/2019MS001663)

Caravelli, F., F. C. Sheldon and F. L. Traversa. Global minimization via classical tunneling assisted by collective force field formation. 2021. *Science Advances*. **7** (52): eabh1542. (LA-UR-21-20810 DOI: 10.1126/sciadv.abh1542)

Caravelli, F., M. D. Saccone, K. Hofhuis, S. Parchenko, Y. A. Birkh\xc3\xb6lzer, S. Dhuey, A. K. Kleibert, S. van Dijken, C. Nisoli and A. Farhan. Direct observation of a dynamical glass transition in a nanomagnetic artificial Hopfield network. Submitted to *Nature Physics*. (LA-UR-21-28829)

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

*Cheng, W., W. Weijer, W. M. Kim, G. Danabasoglu, S. G. Yeager, P. R. Gent, D. Zhang, J. C. H. Chiang and J. Zhang. Can the Salt-Advection Feedback Be Detected in Internal Variability of the Atlantic Meridional Overturning Circulation?. 2018. *Journal of Climate*. **31** (16): 6649-6667. (LA-UR-18-21355 DOI: 10.1175/JCLI-D-17-0825.1)

Ecke, R. E., O. Shishkina and X. Zhang. Boundary zonal flows in rapidly rotating turbulent thermal convection. Submitted to *Journal of Fluid Mechanics*. (LA-UR-20-27752)

Ecke, R. E., X. Zhang and O. Shishkina. Where have all the wall modes gone? Rethinking rotating Rayleigh-B\xc3\xa9nard convection in the geostrophic regime. Submitted to *Physical Review Letters*. (LA-UR-21-26526)

*Gu, S., Z. Liu, A. Jahn, J. Rempfer, J. Zhang and F. Joos. Modeling Neodymium Isotopes in the Ocean Component of the Community Earth System Model (CESM1). 2019. *Journal of Advances in Modeling Earth Systems*. **11** (3): 624-640. (LA-UR-19-21453 DOI: 10.1029/2018MS001538)

*Gu, S., Z. Liu, J. Lynch-Stieglitz, A. Jahn, J. Zhang, K. Lindsay and L. Wu. Assessing the Ability of Zonal \xce\xb4 O Contrast in Benthic Foraminifera to Reconstruct Deglacial Evolution of Atlantic Meridional Overturning Circulation. 2019. *Paleoceanography and Paleoclimatology*. **34** (5): 800-812. (LA-UR-19-25176 DOI: 10.1029/2019PA003564)

*Hecht, M., M. Veneziani, W. Weijer, B. Kravitz, S. Burrows, D. Comeau, E. Hunke, N. Jeffery, J. Urrego-Blanco, W. Hailong, W. Shanlin, Z. Jiaxu, D. Bailey, C. Mills, P. Rasch and N. Urban. E3SMv0-HiLAT: A Modified Climate

System Model Targeted for the Study of High-Latitude Processes. 2019. *Journal of Advances in Modeling Earth Systems*. **11** (8): 2814-2843. (LA-UR-18-27813 DOI: 10.1029/2018MS001524)

Hofhuis, K., C. F. Petersen, M. D. Saccone, S. Dhuey, A. Kleibert, S. van Dijken and A. Farhan. Geometrically frustrated kagome-triangular lattice: ice-rule vs. vortex-driven order. Submitted to *Physical Review B*. (LA-UR-21-23310)

Ma, T., H. Kim, N. Mathew, D. J. Luscher, L. Cao and A. Hunter. Dislocation transmission across \xce\xa33{112} incoherent twin boundary: a combined atomistic and phase-field study. Submitted to *Acta Materialia*. (LA-UR-21-23403)

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

Miller, J. M., T. M. Sprouse, C. L. Fryer, B. R. Ryan, J. C. Dolence, M. R. Mumpower and R. A. Surman. Full Transport General Relativistic Radiation Magnetohydrodynamics for Nucleosynthesis in Collapsars. Submitted to *Astrophysical Journal*. (LA-UR-19-30392)

*Peng, X., N. Mathew, I. J. Beyerlein, K. Dayal and A. Hunter. A 3D phase field dislocation dynamics model for body-centered cubic crystals. 2020. *Computational Materials Science*. **171**: 109217. (LA-UR-19-24421 DOI: 10.1016/j.commatsci.2019.109217)

Saccone, M. D., F. Caravelli, K. Hofhuis, S. Parchenko, S. Dhuey, A. Kleibert, C. Nisoli and A. Farhan. Direct observation of a dynamical glass transition in a nanomagnetic artificial Hopfield network. Submitted to *Nature Physics*. (LA-UR-21-27055)

*. L. H. *. F. K. A. Sadler, J. D., J. D. Sadler, H. Li and K. A. Flippo. Parameter space for magnetization effects in high-energy-density plasmas. 2021. *Matter and Radiation at Extremes*. **6** (6): 65902. (LA-UR-21-23302 DOI: 10.1063/5.0057087)

*Sadler, J. D., C. A. Walsh and H. Li. Symmetric Set of Transport Coefficients for Collisional Magnetized Plasma. 2021. *Physical Review Letters*. **126** (7): 075001. (LA-UR-20-26919 DOI: 10.1103/PhysRevLett.126.075001)

*Sadler, J. D. and H. Li. Thermomagnetic instability of plasma composition gradients. 2020. *Physics of Plasmas*. **27** (12): 122110. (LA-UR-20-26924 DOI: 10.1063/5.0027210)

Sornborger, A. T., A. F. M. V. Renner, F. C. Sheldon and A. V. Zlotnik. The Backpropagation Algorithm Implemented on Spiking Neuromorphic Hardware. Submitted to *Nature Machine Intelligence*. (LA-UR-21-24457)

Sweeney, M. R., C. W. Gable, S. Karra, P. H. Stauffer, R. J. Pawar and J. D. Hyman. Upscaled discrete fracture matrix model (UDFM): an octree-refined continuum representation of fractured porous media. Submitted to *Computational Geosciences*. (LA-UR-19-25805)

*Sweeney, M. R. and J. D. Hyman. Stress Effects on Flow and Transport in Three-Dimensional Fracture Networks. 2020. *Journal of Geophysical Research: Solid Earth*. **125** (8): e2020JB019754. (LA-UR-19-30234 DOI: 10.1029/2020JB019754)

*Tews, I., J. Margueron and S. Reddy. Confronting gravitational-wave observations with modern nuclear physics constraints. 2019. *The European Physical Journal A*. **55** (6): 97. (LA-UR-19-20198 DOI: 10.1140/epja/i2019-12774-6)

*Thibodeau, B., C. Not, J. Hu, A. Schmittner, D. Noone, C. Tabor, J. Zhang and Z. Liu. Last Century Warming Over the Canadian Atlantic Shelves Linked to Weak Atlantic Meridional Overturning Circulation. 2018. *Geophysical Research Letters*. **45** (22): 12. (LA-UR-19-21455 DOI: 10.1029/2018GL080083)

Tynes, M. F., W. Gao, D. J. Burrill, E. R. Batista, D. Perez, P. Yang and N. E. Lubbers. Pairwise difference regression: a machine learning meta-algorithm for improved prediction and uncertainty quantification in chemical search. Submitted to *Journal of Chemical Information and Modeling*. (LA-UR-21-21066)

Walsh, C. A., J. D. Sadler and J. R. Davies. Impact of Updated Extended-MHD Transport Coefficients on Laboratory Plasmas. Submitted to *High Energy Density Physics*. (LA-UR-21-24909)

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

Wang, K., Y. Chen, M. Z. S. Mehana, N. E. Lubbers, K. Bennett, Q. Kang, H. S. Viswanathan and T. C. Germann. A physics-informed and hierarchically regularized data-driven model for predicting fluid flow through porous media. Submitted to *Journal of Computational Physics*. (LA-UR-20-27444)

*Weijer, W., W. Cheng, S. S. Drijfhout, A. V. Fedorov, A. Hu, L. C. Jackson, W. Liu, E. L. McDonagh, J. V. Mecking and J. Zhang. Stability of the Atlantic Meridional Overturning Circulation: A Review and Synthesis. 2019. *Journal of Geophysical Research: Oceans*. **124** (8): 5336-5375. (LA-UR-19-21448 DOI: 10.1029/2019JC015083)

Yakymenko, K., J. E. Borovsky and G. L. Delzanno. Modification of the Loss Cone for Energetic Particles in the Earth's Inner Magnetosphere. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-21-30936)

Zhang, D. Z., G. Akiki, R. M. Rauenzahn and M. M. Francois. Particle-fluid-particle Stress in Disperse Multiphase Flows. Submitted to *Journal of Fluid Mechanics*. (LA-UR-18-30169)

Reports

Akiki, G. and D. Z. Zhang. NUMERICAL INVESTIGATION OF THE DRAG ON A SHOCK ACCELERATED PARTICLE. Unpublished report. (LA-CP-18-20833)

Russell, C. S. Carbon Capture and Synergistic Energy Storage: Performance and Uncertainty Quantification. Unpublished report. (LA-UR-19-21781)

Sadler, J. D. Theoretical justification for heat flux limiter 0.15. Unpublished report. (LA-UR-21-24977)

Zhang, J., W. Weijer, M. E. Maltrud, C. Veneziani, N. Jeffery, E. C. Hunke, J. R. Urrego Blanco and J. D. Wolfe. An eddy-permitting ocean-sea ice general circulation model (E3SMv0-HiLAT03): Description and evaluation. Unpublished report. (LA-UR-19-25177)

Presentation Slides

Akiki, G., M. M. Francois and D. Z. Zhang. Particle-Fluid-Particle Stress in Multiphase Flows. Presented at *American Physical Society Division of Fluid Dynamics*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-30873)

Andrews, E. M., J. D. Hyman, M. R. Sweeney, J. D. Moulton and A. Navarre-Sitchler. Elucidating the effect of subsurface structure on mineral dissolution rates using reactive transport modeling. Presented at *Goldschmidt Conference*, Virtual, Colorado, United States, 2021-07-05 - 2021-07-09. (LA-UR-21-25963)

Banerjee, S. Theory and modeling of quantum mechanical transport for electron and negative-ion sources. Presented at *2021 Virtual theoretical Division Lightning Talks*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-28017)

Banerjee, S., A. Piryatinski, T. J. T. Kwan, P. Zhang and C. Huang. Transverse properties of the electron beam emitted from a diamond nanotip. Presented at *Photocathode Physics for Photoinjectors Workshop 2021*, Melno Park, California, United States, 2021-11-10 - 2021-11-12. (LA-UR-21-31112)

Chenna, S. P., K. S. B. Cosburn, U. M. Ezeobi and M. Moraru. Optimizing and extending the functionality of EXARL for reinforcement learning. Presented at *LANL Virtual Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-27503)

Curtis, S., J. M. Miller, R. T. Wollaeger, C. Frohlich and N. Wolfe. Core-collapse Supernovae: From Neutrino-Driven 1D Explosions to Light Curves and Spectra. . (LA-UR-20-26964)

DeSantis, D. F., P. J. J. Wolfram and B. Alexandrov. Multiresolution Cluster Analysis - Addressing Trust in Climate Classification. Presented at *AMS Annual Meeting*, Boston, Massachusetts, United States, 2020-01-13 - 2020-01-17. (LA-UR-20-20382)

Garcia, A. E. CNLS Overview Presented to the CNLS External Advisory and LDRD Review Meeting. Presented at *CNLS Review Committee*, Los Alamos, New Mexico, United States, 2021-05-14 - 2021-05-14. (LA-UR-21-24607)

Jadrich, R. B. Accelerating materials design and ab initio simulation via statistical inference and machine learning. . (LA-UR-19-25374)

Mathew, N. Analyzing atomistic simulations of high-strain-rate deformation in metals/high explosives using strain functionals and machine learning. . (LA-UR-18-31489)

Mathew, N. Multi-scale, multi-physics mechanics of engineering materials. . (LA-UR-19-22177)

Miller, J. M. Lessons Learned From Successful Open-Source Projects. Presented at *Deep Learning For Multimessenger Astrophysics*, Urbana, Illinois, United States, 2018-10-17 - 2018-10-17. (LA-UR-18-29778)

Miller, J. M. Accretion, Turbulence, Radiation, and How Machine Learning Can Help. Presented at *Deep Learning for Multimessanger Astrophysics*, Urbana, Illinois, United States, 2018-10-17 - 2018-10-17. (LA-UR-18-29749)

Miller, J. M. and H. Lim. The Sound of Spacetime: Gravitational Waves and What they can Teach us. . (LA-UR-19-30401)

Ramakrishnaiah, V. B., R. S. Pavel and J. Loiseau. Co-Design Summer School. . (LA-UR-21-28912)

Sadler, J. D. Magnetic Field Effects In High Energy Density Plasmas. Presented at *Capability Review - Nuclear and Particle Futures*, Los Alamos, New Mexico, United States, 2021-04-06 - 2021-04-06. (LA-UR-21-23317)

Sadler, J. D., S. Li, S. Green, Y. Lu, K. A. Flippo, H. Li and C. A. Walsh. Symmetric theory of heat and magnetic transport in a collisional magnetized plasma. Presented at *American physical society division of plasma physics conference*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30147)

Sornborger, A. T., A. F. M. V. Renner, F. C. Sheldon, A. V. Zlotnik and L. Tao. A Loihi Implementation of Backpropagation Using Gated Synfire Chains. Presented at *2021 INRC Winter Workshop*, Online, New Mexico, United States, 2021-02-10 - 2021-02-10. (LA-UR-21-21175)

Sornborger, A. T., A. F. M. V. Renner, F. C. Sheldon, L. Tao and A. V. Zlotnik. The Backpropagation Algorithm Implemented on Spiking Neuromorphic Hardware. Presented at *INRC Weekly Seminar*, Online, New Mexico, United States, 2021-06-16 - 2021-06-16. (LA-UR-21-25666)

Sweeney, M. R. Modeling discrete fracture networks in porous media using a continuum approach. Presented at *Arizona - Los Alamos Days*, Tucson, Arizona, United States, 2019-04-20 - 2019-04-21. (LA-UR-19-23513)

Sweeney, M. R. Leveraging the dfnWorks software suite for continuum modeling of fractured porous media. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29299)

Sweeney, M. R. and J. D. Hyman. How do different stress regimes affect flow and transport in three-dimensional discrete fracture networks?. Presented at *AGU Fall Meeting 2019*, San Francisco, California, United States, 2019-12-08 - 2019-12-14. (LA-UR-19-32163)

Wang, K. Physics-informed deep learning emulator for predicting porous media flow. . (LA-UR-22-22104)

Wang, K., C. W. Johnson, K. Bennett and P. A. Johnson. Transfer learning of instantaneous predictions of fault slow slips from simulation to experiment. Presented at *MMLDT-CSET 2021*, San Diego, California, United States, 2021-09-26 - 2021-09-26. (LA-UR-21-29403)

Wang, K. and K. Bennett. Convolutional Autoencoder (CAE)-based emulator for predicting pore-fluid flow in shale. Presented at *2021 CNLS External Advisory Committee and Review*, Los Alamos, New Mexico, United States, 2021-05-14 - 2021-05-14. (LA-UR-21-24621)

Weijer, W. Viewgraph for Institutional Computing reporting: w20_hilatbg. . (LA-UR-21-21639)

Zhang, D. Z., G. Akik, R. M. Rauenzahn and M. M. Francois. Particle-fluid-particle Interactions in Disperse Multiphase Flow. Presented at *AJKFluids ASME - JSME - KSME Joint Fluids Engineering Conference 2019*, San Francisco, California, United States, 2019-07-29 - 2019-08-01. (LA-UR-19-27223)

Zhang, D. Z., G. Akiki, R. M. Rauenzahn and M. M. Francois. General Definition of Particle-fluid-particle Stress in Multiphase Flows. Presented at *APS/DFD*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-30757)

Zhang, J. The role of the Beaufort Gyre in Arctic and global climate variability: An eddy-permitting ocean-sea ice model perspective (w18_hilatbg). . (LA-UR-19-21748)

Zhang, J., W. Weijer, M. Steele, W. Cheng and T. Verma. Impact of the Beaufort Gyre freshwater release on deepwater formation in the North Atlantic. Presented at *2020 Ocean Sciences Meeting*, San Diego, California, United States, 2020-02-16 - 2020-02-21. (LA-UR-20-21349)

Posters

Andrews, E. M., M. R. Sweeney, J. D. Moulton, A. Navarre-Sitchler and J. D. Hyman. Simulating Mineral Weathering in 3D Fractured Media. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29542)

Chenna, S. P., K. S. B. Cosburn, U. M. Ezeobi, M. Moraru, H. Lim, J. Loiseau, J. Mohd-Yusof, R. S. Pavel, V. B. Ramakrishnaiah, A. R. Reisner and K. C. Tsai. Optimizing and Extending the Functionality of EXARL for Scalable Reinforcement Learning. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis*, St Louis, Missouri, United States, 2021-11-14 - 2021-11-14. (LA-UR-21-27793)

Jadrich, R. B. Accelerating reactive ab initio simulation via Nested Monte Carlo and Machine Learning. . (LA-UR-19-24686)

Pal, N., S. Kurien, D. Aslangil, D. Livescu and T. T. Clark. Understanding the physics of turbulent mixing : a study of two-point correlation functions. Presented at *Arizona - Los Alamos Days*, Tuscon, Arizona, United States, 2019-04-20 - 2019-04-21. (LA-UR-19-23483)

Sadler, J. D., C. A. Walsh, H. Li and K. A. Flippo. Movement of magnetic fields in a collisional plasma. Presented at *Omega laser user group meeting*, Online, NM, New Mexico, United States, 2021-04-27 - 2021-04-30. (LA-UR-21-23514)

Sweeney, M. R. and J. D. Hyman. How do different stress regimes affect transport in three-dimensional discrete fracture networks?. Presented at *LANL Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28466)

Sweeney, M. R. and J. D. Hyman. How do different stress networks affect transport in three-dimensional discrete fracture networks?. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29295)

Zhang, J., W. Weijer, W. Cheng, M. Steele and T. Verma. The release routes of the Beaufort Gyre freshwater and its impact on the North Atlantic. Presented at *2019 AGU Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31913)

Other

Piotrowska-Karpov, J. and J. M. Miller. Pseudospectral Shock Capturing for the Euler Equations. Dataset. (LA-UR-21-30794)

Weijer, W. and J. Zhang. CORE inter-annual forced ocean ice simulation using E3SMv0-HiLAT-tx0.3v2 (HiLAT03). Dataset. (LA-UR-20-25544)

Wu, S., P. Yang and D. Perez. Abstract for the dataset "Dataset of accelerated molecular dynamics simulations of Thorium Oxide nanoparticles". Dataset. (LA-UR-20-24609)

Information Science and Technology

Quantum Chemistry using Quantum Computers

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Project Description

Quantum computers (QC) promise to be a game changer for materials science modeling, an appropriate implementation, but the tools are yet to be developed. Hybrid quantum-classical algorithms are the current state-of-the-art in the noisy intermediate-state quantum (NISQ) era. Existing advances such as variational quantum eigensolver (VQE) solvers need quality initial states (ansatzes) and minimal number of qubits for each problem at hand (currently limited to very small molecules only). Subsequently, casting the original problems in terms of novel Information Science and Technology (IS&T) algorithms and software layers is a key ingredient for solving the quantum problem and demonstrating practical utility of existing QC hardware. Our particular innovation is the development of algorithms able to achieve the qubit size reduction for quantum solver methods based on Machine Learning, Quantum Graph Partitioning, High-Performance Computing (HPC) and Quantum Computing unique to Los Alamos National Laboratory and without sacrificing accuracy. This project is delineated into three distinct tasks: 1) develop strategies and algorithms to perform static quantum chemistry calculations on medium-to-large size molecules on QCs; 2) develop quantum molecular dynamics on QCs; 3) extend algorithms to excited states and non-equilibrium molecular dynamics beyond the Born-Oppenheimer approximation.

Publications

Journal Articles

Arrasmith, A. T., L. Cincio, R. D. Somma and P. J. Coles. Operator Sampling for Shot-frugal Optimization in Variational Algorithms. Submitted to *npj Quantum Information*. (LA-UR-20-22810)

Bilkis, M., M. V. S. Cerezo de la Roca, G. Verdon, P. J. Coles and L. Cincio. A semi-agnostic ansatz with variable structure for quantum machine learning. Submitted to *Quantum*. (LA-UR-21-22040)

Cincio, L., N. Tkachenko, J. P. Sud, Y. Zhang, S. Tretiak, P. M. Anisimov, A. T. Arrasmith, P. J. Coles and P. Dub. Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in VQE. Submitted to *PRX quantum, arxiv*. (LA-UR-20-26797)

A. A. *. C. P. J. *. C. L. Czarnik, P. *., P. J. Coles, L. Cincio, P. Czarnik and A. Arrasmith. Error mitigation with Clifford quantum-circuit data. 2021. *Quantum*. **5**: 592. (LA-UR-20-23755 DOI: 10.22331/q-2021-11-26-592)

Dub, P. Homochiral \xce\xb2-CF3, -SCF3 and -OCF3 secondary alcohols: catalytic stereoconvergent synthesis, bioactivity and flexible crystals. Submitted to *JACS*. (LA-UR-22-21454)

*Dub, P., R. J. Batrice, J. C. Gordon, B. L. Scott, Y. Minko, J. G. Schmidt and R. F. Williams. Engineering Catalysts for Selective Ester Hydrogenation. 2020. *Journal of the American Chemical Society*. **24** (3): 415-442. (LA-UR-19-31371 DOI: 10.1021/acs.oprd.9b00559)

Gayday, I., D. Babikov, A. Teplukhin, B. K. Kendrick, S. M. Mniszewski, C. F. A. Negre, Y. Zhang, S. Tretiak and P. Dub. Molecular Dynamics Simulations on Quantum Annealers. Submitted to *Nature Communications*. (LA-UR-21-30156)

*Kuebler, J. M., A. Arrasmith, L. Cincio and P. J. Coles. An Adaptive Optimizer for Measurement-Frugal Variational Algorithms. 2020. *Quantum*. **4**: 263. (LA-UR-19-29383 DOI: 10.22331/q-2020-05-11-263)

Lee, S., J. Lee, H. Zhai, Y. Tong, A. M. Dalzell, A. Kumar, P. Helms, J. Gray, M. Kastoryano, R. Babbush, D. R. Reichman, E. T. Campbell, E. F. Valeev, L. Lin and G. K. Chan. Is there exponential quantum advantage in quantum chemistry?. Submitted to *Nature*. (LA-UR-22-21175)

Liu, X., A. Angone, R. Shaydulin, I. Safro, Y. Alexeev and L. Cincio. An Approach for Combinatorial Optimization on Noisy Quantum Computers. Submitted to *quantum science & technology arxiv*. (LA-UR-21-20623)

Mniszewski, S. M., P. D. Akrobotu, T. E. James and C. F. A. Negre. A QUBO Formulation for Eigencentralit. Submitted to *Quantum Information Processing*. (LA-UR-21-24030)

Mniszewski, S. M., P. Dub, S. Tretiak, P. M. Anisimov, Y. Zhang and C. F. A. Negre. Downfolding the Molecular Hamiltonian Matrix using Quantum Community Detection. Submitted to *Nature Communications*. (LA-UR-20-26971)

A. Negre, C. F., A. Lopez-Bezanilla, Y. Zhang, P. Akrobotu, S. M. Mniszewski, S. Tretiak and P. Dub. QUBO-based density matrix electronic structure method. Submitted to *JCTC*. (LA-UR-22-20271)

*Reinaudi, L., C. F. Negre and M. C. Gimenez. Monte Carlo simulations for understanding the transport properties of metallic nanowires. 2020. *Physica E: Low-dimensional Systems and Nanostructures*. **124**: 114326. (LA-UR-20-24467 DOI: 10.1016/j.physe.2020.114326)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio and P. J. Coles. Variational Quantum Algorithms. Submitted to *Nature Reviews Physics*. (LA-UR-20-30142)

*K. B. K. *. M. S. M. *. Z. Y. *. K. A. *. N. C. F. A. *. A. P. M. *. T. S. *. D. P. A. Teplukhin, A. *., A. Teplukhin, B. K. Kendrick, S. M. Mniszewski, A. Kumar, C. F. A. Negre, P. M. Anisimov, S. Tretiak, Y. Zhang and P. A. Dub. Computing molecular excited states on a D-Wave quantum annealer. 2021. *Scientific Reports*. **11** (1): 18796. (LA-UR-21-25914 DOI: 10.1038/s41598-021-98331-y)

Teplukhin, A., B. K. Kendrick, S. Tretiak and P. Dub. Electronic structure with direct diagonalization on a D-Wave quantum annealer. Submitted to *Nature Communications*. (LA-UR-20-26844)

Teplukhin, A., B. K. Kendrick, S. Tretiak and P. Dub. Sampling electronic structure QUBOs with Ocean qbsolv and Mukai QUBO solver. Submitted to *Quantum Science and Technology*. (LA-UR-21-20566)

Teplukhin, A., B. K. Kendrick and D. Babikov. Solving complex eigenvalue problems on a quantum annealer with applications to quantum scattering resonances. Submitted to *PCCP. Physical Chemistry Chemical Physics*. (LA-UR-20-26167)

Tretiak, S., B. M. Weight, N. M. S. Khan, B. J. Gifford and A. Bishop. Theoretical study of the optoelectronic properties of Graphene Quantum Dots: different isomers, shapes, and effect of substituents. Submitted to *Journal of Physical Chemistry C*. (LA-UR-22-22436)

Zhang, Y. Theory of Plasmonic Hot-Carrier Generation and Relaxation. 2021. *The Journal of Physical Chemistry A*. **125** (41): 9201-9208. (LA-UR-21-26367 DOI: 10.1021/acs.jpca.1c05837)

Reports

Cincio, L. Error mitigation with Clifford quantum-circuit data. Unpublished report. (LA-UR-22-21698)

Mniszewski, S. M. Combinatorial Optimization and Quantum Chemistry using IBM Q Status Report. Unpublished report. (LA-UR-22-21624)

A. Negre, C. F., B. J. Miller and J. Jimenez-Martinez. A Three-Dimensional Graph-Based Model for Porous Media Fluid Flow. Unpublished report. (LA-UR-21-28145)

Presentation Slides

Arrasmith, A. T., J. Kubler, L. Cincio, R. D. Somma and P. J. Coles. Shot Frugal Optimization for VQE. Presented at *Quantum Techniques in Machine Learning 2020*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-29153)

Cincio, L. Qubit reduction in Electronic Structure Calculations with tensor networks. Presented at *The International Chemical Congress of Pacific Basin Societies (Pacifichem)*, remote, Hawaii, United States, 2021-12-18 - 2021-12-18. (LA-UR-21-32328)

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Dub, P., L. Cincio, S. M. Mniszewski, S. Tretiak, B. K. Kendrick, P. J. Coles, A. Teplukhin, C. F. A. Negre, P. M. Anisimov, N. Tkachenko, A. T. Arrasmith, Y. Zhang and A. Piryatinski. LDRD Project Appraisal 20200056DR. . (LA-UR-20-30228)

Dub, P. and N. Tkachenko. Multiparallel Electronic Structure Simulation. . (LA-UR-21-24369)

Kendrick, B. K. Quantum Chemistry on Quantum Computers: Electronic Structure, Quantum Dynamics, and Collaborations. Presented at *UNLV-QLCI Workshop*, Las Vegas, Nevada, United States, 2019-11-25 - 2019-11-25. (LA-UR-19-31765)

Kumar, A., A. Asthana, C. Masteran, E. F. Valeev, Y. Zhang, L. Cincio, S. Tretiak and P. Dub. Quantum simulation of ground and excited states with a transcorrrelated Hamiltonian: higher accuracy with fewer qubits. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-20 - 2022-03-20. (LA-UR-22-22046)

Lopez-Bezanilla, A. Two-Dimensional Borides Discovery. Presented at *6th IEEE Electron Devices Technology and Manufacturing Conference (EDTM2022).*, Oita, Japan, 2022-03-06 - 2022-03-09. (LA-UR-22-22154)

Mniszewski, S. M. Quantum Chemistry In Pieces. . (LA-UR-20-23201)

Mniszewski, S. M. Quantum Computing Approaches to Graph Partitioning for Electronic Structure Problems. . (LA-UR-20-23202)

Mniszewski, S. M. Quantum Annealing for Chemistry Applications. . (LA-UR-20-24450)

Mniszewski, S. M. Electronic Structure Calculations in Parallel using Quantum Computing. Presented at *ACS Spring 2021 Meeting (Virtual)*, Los Alamos, New Mexico, United States, 2021-04-05 - 2021-04-30. (LA-UR-21-23297)

Mniszewski, S. M. Quantum Community Detection for Reduction of the Molecular Hamiltonian in Electronic Structure Problems. Presented at *ACS Spring 2021 Meeting (Virtual)*,

Los Alamos, New Mexico, United States, 2021-04-05 - 2021-04-30. (LA-UR-21-23769)

Mniszewski, S. M. On the Road to Exascale Computing and Quantum Computing. Presented at *CCS-3 Tech Talk*, Los Alamos, New Mexico, United States, 2021-08-31 - 2021-08-31. (LA-UR-21-28679)

Mniszewski, S. M. Graph Algorithms as Combinatorial Optimization on Quantum Computers. Presented at *2021 IEEE International Conference on Quantum Computing & Engineering (QCE21) Workshop (Virtual)*, Bloomfield, Colorado, United States, 2021-10-18 - 2021-10-22. (LA-UR-21-30334)

Mniszewski, S. M. Quantum Graph Algorithms for Electronic Structure Problems. Presented at *The International Chemical Congress of Pacific Basin Societies (Pacifichem)*, Virtual, New Mexico, United States, 2021-12-16 - 2021-12-21. (LA-UR-21-32179)

Mniszewski, S. M. Combinatorial Optimization and Quantum Chemistry using IBM Q. . (LA-UR-22-21520)

Mniszewski, S. M., J. P. Terry, P. D. Akrobotu and C. F. A. Negre. Quantum Isomer Search on the D-Wave Quantum Annealer. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21873)

Mniszewski, S. M., T. E. James, C. F. A. Negre and P. D. Akrobotu. QCSS Project – Eigenvector Centrality on D-Wave. . (LA-UR-20-26435)

Teplukhin, A., B. K. Kendrick, S. Tretiak and P. Dub. Electronic structure with direct diagonalization on a D \xe2\x80\x91Wave quantum annealer. Presented at *ACS April Meeting 2021 (virtual)*, Washington, District Of Columbia, United States, 2021-04-05 - 2021-04-05. (LA-UR-21-23569)

Teplukhin, A., B. K. Kendrick and D. Babikov. Quantum Annealer Eigensolver (QAE): Combining quantum computing with high-performance computing to solve fundamental chemistry problems. Presented at *The 259th American Chemical Society National Meeting & Exposition (upload to SciMeetings science-sharing platform)*, Philadelphia, Pennsylvania, United States, 2020-03-22 - 2020-03-26. (LA-UR-20-23184)

Tretiak, S. Carbon Nanotubes and Semiconductor Nanocrystals for Quantum Photonics. Presented at *Quantum workshop*, Virtual, New Mexico, United States, 2021-04-19 - 2021-04-19. (LA-UR-21-23728)

Zhang, Y. Quantum Krylov Subspace Method for Excited States. Presented at *2022 APS March meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-19. (LA-UR-22-22012)

Prioritizing the Prior: Advanced Inversion Algorithms for Scientific Data Analysis

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Project Description

There is a diverse range of mission-critical problems both at the Laboratory and within the Department of Energy (DOE) that involve challenging inverse problems with common properties. The full value of the knowledge that can be gained from the experiments depends critically on the effectiveness of the solutions to these inverse problems, which are often very challenging to solve. While there is a wealth of domain expertise at the Laboratory, we have a much more limited capability in the development of the required mathematics and algorithms for solving difficult inverse problems. We propose to establish such a capability, motivated by the recognition that many of the problems that are entirely unrelated from a physics perspective, share significant common properties at the level of the mathematics of inverse problems. This project will develop effective solution-space models that are essential to obtaining reliable solutions of the numerous problems encountered within Laboratory mission areas such as stockpile stewardship, materials science, and energy security. All of these application domains involve very difficult inverse problems for which substantial improvements are expected to be possible, and in some cases, for which there are no current solutions.

Publications

Journal Articles

*SGD-Net: Efficient Model-Based Deep Learning With Theoretical Guarantees. *IEEE Transactions on Computational Imaging*. **7**: 598-610. (LA-UR-21-20696 DOI: 10.1109/TCI.2021.3085534)

Bacak, M., J. Valsecchi, J. Capek, E. Polatidis, A. Kaestner, A. Arabi-Hashemi, I. I. Kruk, C. Leinenbach, A. M. Long, A. S. Tremsin, S. C. Vogel, E. B. Watkins and M. Strobl. Neutron dark-field imaging applied to porosity and deformation-induced phase transitions in additively manufactured steels. Submitted to *Materials & Design*. (LA-UR-20-25975)

Bouman, C. A., G. T. Buzzard and B. E. Wohlberg. Plug and play: a general approach for the fusion of sensor and machine learning models. Submitted to *SIAM News*. (LA-UR-20-28391)

Goyes-Penafiel, P., E. Vargas, C. V. Correa, W. Agudelo, B. E. Wohlberg and H. Arguello. A Consensus Equilibrium Approach for 3D Land Seismic Shots Recovery. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-21-22053)

Hossain, M., B. T. Nadiga, O. Korobkin, M. L. Klasky, J. L. S. Disterhaupt, J. W. Burby, M. T. McCann, T. Wilcox, S. De and C. A. Bouman. High-Precision Inversion of Dynamic Radiography Using Hydrodynamic Features. Submitted to *Optics Express*. (LA-UR-21-31230)

Hovey, L. D. and M. L. Klasky. Parametric Generation of 1D Sedov Point Explosions in Varying Ambient Media using Dynamic Mode Decomposition. Submitted to *Shock Waves*. (LA-UR-21-21016)

Klasky, M. L., Z. HUANG, T. Wilcox and S. Ravishankar. Physics-Driven Learning of Wasserstein GAN for Density Reconstruction in Dynamic Tomography. Submitted to *Optics Express*. (LA-UR-21-30845)

*Lehmann, E. H., D. Mannes, M. Strobl, B. Walfort, A. Losko, B. Schillinger, M. Schulz, S. C. Vogel, D. C. Schaper, D. C. Gautier and D. Newmark. Improvement in the spatial resolution for imaging with fast neutrons. 2021. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **988**: 164809. (LA-UR-20-26818 DOI: 10.1016/j.nima.2020.164809)

*Lin, Y. Data-Driven Seismic Waveform Inversion: A Study on the Robustness and Generalization. 2020. *IEEE Transactions on Geoscience and Remote Sensing*. **58** (10): 6900-6913. (LA-UR-19-24398 DOI: 10.1109/TGRS.2020.2977635)

Lin, Y., J. P. Theiler and B. E. Wohlberg. Physics-Consistent Data-driven Waveform Inversion with Adaptive Data Augmentation. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-20-22488)

Lin, Y., Q. Zeng, S. Feng and B. E. Wohlberg. InversionNet3D:High-Resolution 3D Full Waveform Inversion with Efficient Encoder-Decoder Network. Submitted to *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*. (LA-UR-21-22293)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Connect the Dots: In Situ 4-D Seismic Monitoring of CO_2 Storage With Spatio-Temporal CNNs. 2021. *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-21-22295 DOI: 10.1109/TGRS.2021.3116618)

Lin, Y., S. Feng and B. E. Wohlberg. Multiscale Data-Driven Seismic Full-Waveform Inversion With Field Data Study. 2021. *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-21-20004 DOI: 10.1109/TGRS.2021.3114101)

Losko, A. S., L. L. Daemen, P. Hosemann, H. Nakotte, A. S. Tremsin, S. C. Vogel, P. Wang and F. Wittmann. Separation of Uptake of Water and Ions in Porous Materials using Energy Resolved Neutron Imaging. Submitted to *JOM*. (LA-UR-19-32650)

Losko, A. S. and S. C. Vogel. 3D Isotope Density Measurements by Energy-Resolved Neutron Imaging. Submitted to *Nature*. (LA-UR-19-32651)

*McKeown, M., S. L. Brusatte, T. E. Williamson, J. A. Schwab, T. D. Carr, I. B. Butler, A. Muir, K. Schroeder, M. A. Espy, J. F. Hunter, A. S. Losko, R. O. Nelson, D. C. Gautier and S. C. Vogel. Neurosensory and Sinus Evolution as Tyrannosauroid Dinosaurs Developed Giant Size: Insight from the Endocranial Anatomy of. 2020. *The Anatomical Record*. **303** (4): 1043-1059. (LA-UR-19-32710 DOI: 10.1002/ar.24374)

*Pound, B. A., K. M. Mertes, A. V. Carr, M. H. Seaberg, M. S. Hunter, W. C. Ward, J. F. Hunter, C. M. Sweeney, C. M. Sewell, N. R. Weisse-Bernstein, J. K. S. Baldwin and R. L. Sandberg. Ptychography at the Linac Coherent Light Source in a parasitic geometry. 2020. *Journal of Applied Crystallography*. **53** (5): 1276-1282. (LA-UR-19-32687 DOI: 10.1107/S1600576720010778)

Sun, Y., J. Liu, M. Xie, B. E. Wohlberg and U. S. Kamilov. CoIL: Coordinate-based Internal Learning for Imaging Inverse Problems. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-21-21526)

Sun, Y., Z. Wu, X. Xu, B. E. Wohlberg and U. S. Kamilov. Scalable Plug-and-Play ADMM with Convergence Guarantees. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-20-24233)

Wang, J., B. E. Wohlberg and R. Adamson. Convolutional dictionary learning for blind deconvolution of optical coherence tomography images. Submitted to *Biomedical Optics Express*. (LA-UR-22-21235)

*Wohlberg, B. and P. Wozniak. PSF Estimation in Crowded Astronomical Imagery as a Convolutional Dictionary Learning Problem. 2021. *IEEE Signal Processing Letters*. **28**: 374-378. (LA-UR-20-28195 DOI: 10.1109/LSP.2021.3050706)

Xie, M., Y. Sun, J. Liu, B. E. Wohlberg and U. S. Kamilov. Joint Reconstruction and Calibration Using Regularization by Denoising. Submitted to *IEEE Signal Processing Letters*. (LA-UR-20-29788)

Xu, X., J. Liu, Y. Sun, B. E. Wohlberg and U. Kamilov. Boosting the Performance of Plug-and-Play Priors via Denoiser Scaling. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-19-32413)

*Xu, X., Y. Sun, J. Liu, B. Wohlberg and U. S. Kamilov. Provable Convergence of Plug-and-Play Priors With MMSE Denoisers. 2020. *IEEE Signal Processing Letters*. **27**: 1280-1284. (LA-UR-20-23774 DOI: 10.1109/LSP.2020.3006390)

Yang, H. J., Y. Lin, B. Wohlberg and D. M. Tartakovsky. Consensus Equilibrium for Subsurface Delineation. 2021. *Water Resources Research*. **57** (10): e2021WR030151. (LA-UR-21-24057 DOI: 10.1029/2021WR030151)

Conference Papers

Balke, T., A. M. Long, S. C. Vogel, B. E. Wohlberg and C. A. Bouman. Hyperspectral Neutron Computed Tomography with Material Decomposition. Presented at *2021 IEEE International Conference on Image Processing*. (Anchorage, Alabama, United States, 2021-09-19 - 2021-09-22). (LA-UR-21-21281)

Garcia Cardona, C., R. Kannan, T. Johnston, T. Proffen and S. K. Seal. Structure Prediction from Neutron Scattering Profiles: A Data Sciences Approach. Presented at *2020 IEEE International Conference on Big Data*. (Atlanta, Georgia, United States, 2020-12-10 - 2020-12-10). (LA-UR-21-30158)

Klasky, M. L., A. Lahiri, S. Ravishankar, J. Fessler and T. Wilcox. Limited-View Cone Beam CT Reconstructions using 3D Subvolume-based Supervised and Adversarial Learning: Validation using Hydrodynamic simulations and Experimental Tomographic data. Presented at *2022 Electronic Imaging Symposium*. (San Francisco, California, United States, 2022-01-17 - 2022-01-28). (LA-UR-22-20986)

Klasky, M. L., L. A. Pfister, J. L. S. Disterhaupt, M. T. McCann and S. Ravishankar. Descattering and Reconstruction in MultiMaterial Polyenergetic X-Ray Tomography Using Local Scatter Models. Presented at *OSA Digital Holography and Three-Dimensional Imaging Topical Meeting (DH)*. (Vancover, Canada, 2021-07-19 - 2021-07-19). (LA-UR-21-22245)

Lin, Y., B. E. Wohlberg and J. P. Theiler. Physics-Consistent Data-driven Seismic Inversion with Adaptive Data Augmentation. Presented at *the 34th Conference on Neural Information Processing Systems (NeurIPS)*. (Vancouver, Canada, 2020-12-06 - 2020-12-06). (LA-UR-20-27731)

Lin, Y., J. D. Moulton, B. E. Wohlberg, E. Cromwell and X. Chen. CycleFCN: A Physics-Informed Data-driven SeismicWaveform Inversion. Presented at *Society of Exploration Geophysics Annual Meeting*. (houston, Texas, United States, 2020-10-11 - 2020-10-11). (LA-UR-20-22907)

Lin, Y., Q. Zeng, S. Feng and B. E. Wohlberg. 3D FullWaveform Inversion via Deep Encoder-Decoder Networks. Presented at *SEG 2021 Annual Meeting*. (denver, Colorado, United States, 2021-09-26 - 2021-09-26). (LA-UR-21-23217)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Monitoring and Forecasting CO_2 Storage in the Sleipner area with Spatio-temporal CNNs. Presented at *SEG 2021 Annual Meeting*. (denver, Colorado, United States, 2021-09-26 - 2021-09-26). (LA-UR-21-23218)

Lin, Y. and B. E. Wohlberg. Physically Realistic Training Data Building for Data-driven Full-waveform Inversion and Traveltime Tomography. Presented at *Society of Exploration Geophysics Annual Meeting*. (houston, Texas, United States, 2020-10-11 - 2020-10-11). (LA-UR-20-22908)

Lin, Y. and B. E. Wohlberg. How Good Is Your Scientific Data Generative Model?. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*. (denver, Colorado, United States, 2020-11-15 - 2020-11-15). (LA-UR-20-27518)

Liu, J., M. S. Asif, B. E. Wohlberg and U. S. Kamilov. Recovery Analysis for Plug-and-Play Priors using the Restricted Eigenvalue Condition. Presented at *Neural Information Processing Systems*. (Vancouver, Canada, 2021-12-06 - 2021-12-06). (LA-UR-21-25612)

Lu, J., Y. Sun, W. Gan, X. Xu, B. E. Wohlberg and U. S. Kamilov. Stochastic Deep Unfolding for Imaging Inverse Problems. Presented at *2021 IEEE International Conference on Acoustics, Speech and Signal Processing*. (Toronto, Canada, 2021-06-06 - 2021-06-06). (LA-UR-20-27581)

Sun, Y., J. Liu, Y. Sun, B. E. Wohlberg and U. S. Kamilov. Async-RED: A Provably Convergent Asynchronous Block Parallel Stochastic Method using Deep Denoising Priors. Presented at *International Conference on Learning Representations*. (Vienna, Austria, 2021-05-04 - 2021-05-04). (LA-UR-20-28190)

Zhai, Q., B. E. Wohlberg, G. Buzzard and C. Bouman. Projected Multi-Agent Consensus Equilibrium for Ptychographic Image Reconstruction. Presented at *Asilomar Conference on Signals, Systems, and Computers*. (Asilomar, California, United States, 2021-10-31 - 2021-10-31). (LA-UR-21-32031)

Reports

Klasky, M. L., B. T. Nadiga, J. L. S. Disterhaupt, E. Guardincerri, J. L. Carroll, L. A. Pfister, L. D. Hovey, E. W. Skau, G. P. Salazar, B. J. Warthen, A. J. Mendez, M. E. Schulze, J. E. Coleman, C. R. Rose, M. A. Espy, B. E. Wohlberg, Y. Han, T. Wilcox, T. Mockler, A. L. Hungerford, S. Ravishankar, M. McCann, Y. Bresler, B. Iskender, A. Lahiri and C. Bouman. Hydrodynamic and Radiographic Toolbox (HART). Unpublished report. (LA-UR-20-24084)

Klasky, M. L., B. T. Nadiga, J. L. S. Disterhaupt, T. Wilcox, L. D. Hovey, T. Mockler, C. L. Fryer, E. N. Loomis, A. L. Hungerford, S. K. Sjue, L. A. Pfister and Y. Han. UNCERTAINTIES IN DENSITY AND SIMULATION PARAMETERS FOR RADIOGRAPHIC RECONSTRUCTIONS USING MACHINE LEARNING. Unpublished report. (LA-UR-20-24065)

Vogel, S. C., T. Balke, C. A. Bouman, L. Capriotti, J. M. Harp, A. M. Long, D. Schaper, A. S. Tremsin and B. E. Wohlberg. First Examination of Irradiated Fuel with Pulsed Neutrons at LANSCE – Preliminary Results. Unpublished report. (LA-UR-20-27504)

Vogel, S. C., T. Balke, C. A. Bouman, L. Capriotti, J. M. Harp, A. M. Long and B. E. Wohlberg. Characterization of an Irradiated U-1Pd-10Zr Fuel Sample (AFC-3A-R5) with Pulsed Neutrons. Unpublished report. (LA-UR-21-29144)

Vogel, S. C. and E. B. Watkins. Neutron Imaging Using Grating Interferometry: Exploiting phase contrast and dark-field imaging for <1\xce\xbcm feature detection in bulk materials. Unpublished report. (LA-UR-20-27576)

Presentation Slides

Balke, T., A. M. Long, S. C. Vogel, B. E. Wohlberg and C. A. Bouman. Transmission Spectrum Estimation and Material Decomposition with Energy Resolved Neutron Imaging. Presented at *2021 TMS Annual Meeting & Exhibition*, Orlando, Florida, United States, 2021-03-14 - 2021-03-18. (LA-UR-21-22114)

Balke, T., A. M. Long, S. C. Vogel, B. E. Wohlberg and C. A. Bouman. Hyperspectral Neutron Computed Tomography. . (LA-UR-21-24440)

Balke, T., A. M. Long, S. C. Vogel, B. E. Wohlberg and C. A. Bouman. Hyperspectral Neutron CT with Material Decomposition. Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2022-01-11 - 2022-01-11. (LA-UR-22-20117)

Garcia Cardona, C. Advanced Inversion Algorithms for Scientific Data Analysis. . (LA-UR-21-21830)

Garcia Cardona, C., B. E. Wohlberg and Y. Sun. Learning Convolutional Sparse Representations. Presented at *Join Mathematics Meetings*, Denver, Colorado, United States, 2020-01-15 - 2020-01-18. (LA-UR-20-20492)

Garcia Cardona, C., R. Kannan, T. Johnston, T. Proffen and S. K. Seal. Structure Prediction from Neutron Scattering Profiles: A Data Sciences Approach. Presented at *IEEE BigData 2020*, Virtual Conference, New Mexico, United States, 2020-12-10 - 2020-12-13. (LA-UR-20-29777)

Hossain, M., M. L. Klasky, B. T. Nadiga, O. Korobkin, J. L. S. Disterhaupt, J. W. Burby, T. Wilcox, S. De, C. Bouman and M. T. McCann. Physics based Learning from Hydrodynamics Simulations with Mass Constraints for Density Reconstruction in Dynamic Tomography. Presented at *Electronic Imaging 2022*, San Francisco, California, United States, 2022-01-17 - 2022-01-28. (LA-UR-22-20738)

Klasky, M. L., B. T. Nadiga, M. Hossain, O. Korobkin, J. L. S. Disterhaupt, M. T. McCann, Z. Huang, J. Fessler, S. Ravishankar and A. Lahiri. Overview of Physics Informed Dynamic Radiography FY22 Progress. Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2022-01-11 - 2022-01-11. (LA-UR-22-20148)

Klasky, M. L., C. Bouman, J. L. S. Disterhaupt, M. A. Espy, J. Fessler, M. Hossein, E. Guardincerri, L. D. Hovey, O. Korobkin, A. Lahiri, M. McCann, B. T. Nadiga, B. M. Patterson, L. A. Pfister, S. K. Sjue, S. Ravishankar, D. L. Sanzo, T. Wilcox and B. E. Wohlberg. EREBUS Coupled Hydrodynamic Radiographic Dynamic Reconstruction & Limited View Reconstructions. . (LA-UR-21-22694)

Klasky, M. L., C. Bouman, J. L. S. Disterhaupt, O. Korobkin, M. Hossein, L. D. Hovey, M. McCann, B. T. Nadiga, L. A. Pfister, S. Ravishankar, T. Wilcox, B. E. Wohlberg and D. L. Sanzo. Physics Informed Dynamic Radiography. Presented at *LDRD FY Review*, Los Alamos, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30149)

Klasky, M. L., M. Hossain, C. Bouman, J. L. S. Disterhaupt, T. Wilcox, O. Korobkin and L. D. Hovey. Coupled Hydrodynamic & Radiographic Reconstruction using Physics based Machine Learning. Presented at *Dynamic Radiography*, Los Alamos, New Mexico, United States, 2021-04-06 - 2021-04-06. (LA-UR-21-23848)

Klasky, M. L., M. T. McCann, B. E. Wohlberg, M. Hossain, D. L. Sanzo, J. L. S. Disterhaupt, M. A. Espy, O. Korobkin, B. M. Patterson, T. Wilcox, A. Lahiri, J. Fessler, C. Bouman and S. Ravishankar. Dynamic Imaging: Beyond the Standard Model. Presented at *T-Division Student Talk*, Los Alamos, New Mexico, United States, 2021-07-22 - 2021-07-22. (LA-UR-21-27913)

Klasky, M. L., M. T. McCann, M. Hossain, D. L. Sanzo, J. L. S. Disterhaupt, O. Korobkin, T. Wilcox, J. W. Burby, S. Majee, A. Lahiri, J. Fessler, C. Bouman and S. Ravishankar. Coupled Hydrodynamic/Radiographic Dynamic Reconstructions: Beyond the Standard Model. Presented at *Enabling 3D mesoscale imaging under dynamic conditions*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-29231)

Klasky, M. L., T. Wilcox, J. L. S. Disterhaupt, Y. Han, L. A. Pfister, S. Ravishankar and M. McCann. Towards a unified radiographic/hydrodynamic approach to obtaining accurate density from dynamic radiographic measurements. Presented at *Dynamic Radiography Introduction*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-18. (LA-UR-20-23590)

Klasky, M. L., Y. Z. Watkins, E. W. Skau, K. A. Stults and L. Hung. MAD using INRAD and Radiography. . (LA-UR-20-21612)

Klasky, M. L., Z. Huang, M. T. McCann, J. L. S. Disterhaupt and S. Ravishankar. Learning from Hydrodynamics Simulations with Mass Constraints for Density Reconstruction in Dynamic Tomography. Presented at *Electronic Imaging 2022*, San Francisco, California, United States, 2022-01-17 - 2022-01-28. (LA-UR-22-20650)

Lin, Y. Advanced Inversion Algorithms for Scientific Data Analysis. . (LA-UR-22-22140)

Lin, Y., D. Coblentz, P. A. Johnson, R. J. Pawar, G. D. J. Guthrie, J. P. Theiler, B. E. Wohlberg, S. Feng and Q. Zeng. Physics-Guided Learning-Driven Computational Seismic Imaging: from Synthetic Practice to Field Applications. Presented at *Machine Learning in Solid Earth Geoscience (Online Seminar Series)*, Los Alamos, New Mexico, United States, 2021-09-10 - 2021-09-10. (LA-UR-21-28839)

Lin, Y., J. P. Theiler and B. E. Wohlberg. Data-driven vs Physics-driven Computational Methods for Large-scale Inverse Problems. Presented at *AGU worrkshop*, San Francisco,, California, United States, 2019-12-08 - 2019-12-08. (LA-UR-19-32196)

Lin, Y., S. Feng, P. Jin, B. E. Wohlberg and J. D. Moulton. CycleFCN: A Physics-Informed Data-driven Seismic Waveform Inversion Method. Presented at *SEG Annual Meeting*, Houston, Texas, United States, 2020-10-12 - 2020-10-12. (LA-UR-20-28299)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Monitoring and Forecasting CO_2 Storage in the Sleipner area with Spatio-temporal CNNs. Presented at *SEG Annual Conference*, denver, Colorado, United States, 2021-09-26 - 2021-09-26. (LA-UR-21-28468)

Lin, Y., S. Feng and B. E. Wohlberg. Physically Realistic Training Data Construction for Data-driven Full-waveform Inversion and Traveltime Tomography. Presented at *Society of Exploration Geophysics Annual Meeting*, Houston, Texas, United States, 2020-10-11 - 2020-10-11. (LA-UR-20-26781)

Lin, Y., Y. Yang and B. E. Wohlberg. How Good Is Your Scientific Data Generative Model?. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*, denver, Colorado, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-27918)

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

Vogel, S. C., A. M. Long, D. C. Gautier, J. Valloton and H. Henein. Neutron and X-ray Characterization of D2 Tool Steel Solidified in Microgravity. Presented at *Center for Space and Earth Science Microgravity Symposium*, los alamos, New Mexico, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28477)

Vogel, S. C., J. R. Angell, T. Balke, D. T. Carver, L. Capriotti, A. E. Craft, J. Harp, P. Hosemann, J. Lin, A. M. Long, E. J. Larson, K. J. Mcclellan and D. Schaper. Characterization of Irradiated Nuclear Fuels with Pulsed Neutrons. Presented at *TMS Annual Meeting*, virtual, New Mexico, United States, 2021-03-14 - 2021-03-14. (LA-UR-21-22081)

Wohlberg, B. E., C. Garcia Cardona, S. C. Vogel, T. Balke, A. M. Long, M. L. Klasky, K. M. Mertes, J. L. Barber, Y. Lin, L. A. Pfister, S. Feng, O. Korobkin and J. F. Hunter. LDRD Project 20200061DR Review. . (LA-UR-20-30159)

Wohlberg, B. E. and P. R. Wozniak. A Global Optimization
    Approach to PSF Estimation in Crowded Astronomical
    Imagery. . (LA-UR-21-24756)

Wohlberg, B. E. and P. R. Wozniak. A Global Optimization
    Approach to PSF Estimation in Crowded Astronomical
    Imagery. Presented at *OSA Imaging and Applied Optics
    Congress*, Online, California, United States, 2021-07-19 -
    2021-07-19. (LA-UR-21-26815)

In-Situ Inference: Bringing Advanced Data Science into Exascale Simulations

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Project Description

Predictive simulations on large-scale supercomputers are at the heart of computational science in a range of mission areas spanning energy, nuclear stockpile stewardship, and physical and biological science and engineering. Modern high performance computing architectures now generate far more scientific data than can be saved to disk for later analysis, leading to a potential crisis in our ability to understand and use the predictions of scientific models. This requires moving the analysis into the simulation itself, "in-situ". Advanced statistical analysis, or "inference", methods are currently not designed to scale to in-situ deployment within Department of Energy exascale supercomputers. We will develop new parallel statistical algorithms capable of analyzing vast quantities of spatial and time varying data as they are being generated by physics simulations. This will enable an unprecedented level of detail in our ability to analyze the highly complex phenomena that exascale models will simulate, such as the risk and causes of rare, high-impact events such as winter storms or solar-geomagnetic space hazards.

Publications

Journal Articles

Banesh, D., N. Panda, A. Biswas, L. Van Roekel, D. A. Oyen, N. M. Urban and E. C. Lawrence. Fast GP Estimation for In-situ Inference using Convolutional Neural Networks. Submitted to *Machine Learning with Applications*. (LA-UR-21-28495)

Bhowmick, R., J. C. Trepanier and A. M. Haberlie. Southwest Pacific Tropical Cyclone Development Classification Utilizing Machine Learning and Synoptic Composites. 2021. *International Journal of Climatology*. (LA-UR-21-31103 DOI: 10.1002/joc.7457)

Biswas, A., S. Dutta, E. Lawrence, J. Patchett, J. C. Calhoun and J. Ahrens. Probabilistic Data-Driven Sampling via Multi-Criteria Importance Analysis. 2021. *IEEE Transactions on Visualization and Computer Graphics*. **27** (12): 4439-4454. (LA-UR-20-20029 DOI: 10.1109/TVCG.2020.3006426)

Grosskopf, M. J., E. C. Lawrence, K. N. Rumsey, A. Biswas and N. Urban. Estimating a Spatial Inference Model to a Climate Simulation In-Situ with Sparse Gaussian Processes. Submitted to *ISAV 2021: In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization Proceedings*. (LA-UR-21-28251)

Katzfuss, M., J. Guinness and E. C. Lawrence. Scaled Vecchia approximation for fast computer-model emulation. Submitted to *Technometrics*. (LA-UR-20-23222)

Moran, K. R. and M. W. Wheeler. Fast increased fidelity samplers for approximate Bayesian Gaussian process regression. Submitted to *Journal of the Royal Statistical Society Series B: Statistical Methodology*. (LA-UR-21-23822)

W. Myren, S. T. and E. C. Lawrence. Comparison of Emulation Techniques for Bayesian Calibration. Submitted to *Statistical Analysis and Data Mining*. (LA-UR-20-25141)

Warr, R. L., D. B. Dahl, J. M. Meyer and A. L. Lui. The Attraction Indian Buffet Distribution. 2021. *Bayesian Analysis*. (LA-UR-21-25718 DOI: 10.1214/21-BA1279)

Conference Papers

Dutta, S., N. E. Klein, L. Tang, J. D. Wolfe, L. Van Roekel, A. Biswas, N. Urban and E. C. Lawrence. In Situ Climate Modeling for Analyzing Extreme Weather Events. Presented at *ISAV 2021: In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization*. (St. Louis, Missouri, United States, 2021-11-15 - 2021-11-15). (LA-UR-21-28289)

Hazarika, S., A. Biswas, E. C. Lawrence and P. J. J. Wolfram. Probabilistic Principal Component Analysis Guided Spatial Partitioning of Multivariate Ocean Biogeochemistry Data. Presented at *Visualization in Environmental Sciences 2021 (EnvirVis 2021)*. (Zurich, Switzerland, 2021-06-14 - 2021-06-14). (LA-UR-21-22299)

Hazarika, S., A. Biswas, P. J. J. Wolfram, E. C. Lawrence and N. M. Urban. Relationship-aware Multivariate Sampling Strategy for Scientific Simulation Data. Presented at *IEEE Visualization Conference 2020*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-20-24913)

Lawrence, E. C., A. Biswas and N. Urban. In Situ Inference. Presented at *AI@DOE*. (Online, New Mexico, United States, 2021-12-09 - 2021-12-09). (LA-UR-21-31718)

Wang, Y., N. E. Klein, S. K. Morley, V. K. Jordanova, M. G. Henderson, A. Biswas and E. C. Lawrence. TributaryPCA: Distributed, Streaming PCA for In Situ Dimension Reduction with Application to Space Weather Simulations. Presented at *The 7th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-7)*. (St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14). (LA-UR-21-28545)

Reports

Biswas, A., H. W. Shen, J. M. Miller and C. L. Fryer. Machine Learning for Extreme-Scale Particle Data Visualization. Unpublished report. (LA-UR-21-32118)

Biswas, A. and E. C. Lawrence. Annual Report for w20_insituinf, year 2021. Unpublished report. (LA-UR-22-21694)

Lawrence, E. C., A. Biswas, L. Van Roekel and N. Urban. In Situ Inference for Earth System Predictability. Unpublished report. (LA-UR-21-21483)

Urban, N. M., E. C. Lawrence and A. Biswas. In-Situ Inference: Bringing Advanced Data Science Into Exascale Simulations. Unpublished report. (LA-UR-20-20586)

Presentation Slides

Banesh, D. IEEE 2022 SciVis Contest. Presented at *IEEE Vis 2022*, Oklahoma City, Oklahoma, United States, 2022-10-23 - 2022-10-23. (LA-UR-21-30413)

Banesh, D. Topological Data Analysis for Space Weather Modeling. Presented at *IEEE Big Data*, Los Alamos, New Mexico, United States, 2021-12-15 - 2021-12-15. (LA-UR-21-31617)

Banesh, D. Fast Gaussian Process Estimation for Large-Scale In Situ Inference using Convolutional Neural Networks. Presented at *IEEE Big Data Conference*, Los Alamos, New Mexico, United States, 2021-12-15 - 2021-12-15. (LA-UR-21-31618)

Banesh, D., N. Panda, A. Biswas, L. Van Roekel, D. A. Oyen, N. M. Urban, M. J. Grosskopf, J. D. Wolfe and E. C. Lawrence. E3SM/EAM Simulation Data Outputs. Presented at *IEEE Big Data*, Los Alamos, New Mexico, United States, 2021-12-15 - 2021-12-15. (LA-UR-21-31473)

Banesh, D., R. R. Linn and J. M. Patchett. SciVis Contest 2022. Presented at *IEEE Vis 2021*, Los Alamos, New Mexico, United States, 2021-10-24 - 2021-10-24. (LA-UR-21-29624)

Banesh, D., R. R. Linn and J. M. Patchett. Vorticity-Driven Lateral Spread Ensemble Data Set. Presented at *IEEE Vis*, Oklahoma City, Oklahoma, United States, 2022-10-23 - 2022-10-23. (LA-UR-21-30892)

Bhowmick, R., J. J. Benedict, L. Van Roekel, A. Biswas and E. C. Lawrence. Madden-Julian Oscillation Impact on the Probability of Tropical Cyclone Related Extreme Precipitation. Presented at *American Meteorological Society Annual Meeting*, Houston, Texas, United States, 2022-01-23 - 2022-01-27. (LA-UR-22-20651)

Biswas, A. In Situ Data Reduction and Statistical Inference. . (LA-UR-20-30474)

Biswas, A., E. C. Lawrence, M. G. Henderson, V. K. Jordanova, S. K. Morley, N. Panda, M. F. Dorn, M. J. Grosskopf, N. E. Klein, K. N. Rumsey, S. Dutta, S. Hazarika, L. Tang, L. Van Roekel, J. D. Wolfe and N. M. Urban. In-Situ Inference for Exascale Simulations with Julia. Presented at *JuliaCon 2021*, Online, New Mexico, United States, 2021-07-28 - 2021-07-30. (LA-UR-21-26158)

Biswas, A., S. Dutta, E. C. Lawrence, J. M. Patchett, J. C. Calhoun and J. P. Ahrens. Video for talk: "Probabilistic Data-Driven Sampling via Multi-Criteria Importance Analysis". Presented at *IEEE Vis 2021*, Online, Louisiana, United States, 2021-10-24 - 2021-10-24. (LA-UR-21-29110)

Biswas, A. and E. C. Lawrence. CY 2021 Institutional Computing Annual Progress Report. . (LA-UR-22-21629)

Dutta, S. Statistical and Machine Learning Techniques for Enabling Extreme-scale Data Summarization, Feature Exploration, and Visual Analysis. . (LA-UR-21-24331)

Grosskopf, M. J. In Situ Inference for Exascale Scientific Computing. Presented at *Joint Statistical Meeting*, Online, New Mexico, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-25961)

Grosskopf, M. J. In-Situ Spatial Inference on Climate Simulations with Sparse Gaussian Processes. Presented at *ISAV*, Online, New Mexico, United States, 2021-11-15 - 2021-11-15. (LA-UR-21-30615)

Grosskopf, M. J. Distributed, In-Situ Spatial Inference in Climate Simulations with Sparse Gaussian Processes. Presented at *SIAM Conference on Parallel Processing for Scientific Computing*, Online, New Mexico, United States, 2022-02-23 - 2022-02-25. (LA-UR-22-21535)

Hazarika, S., A. Biswas, E. C. Lawrence and P. J. J. Wolfram. Probabilistic Principal Component Analysis Guided Spatial Partitioning of Multivariate Ocean Biogeochemistry Data. Presented at *Visualization in Environmental Sciences 2021 workshop, co-located with EuroVis 2021 (VIRTUAL)*, zurich, Switzerland, 2021-06-14 - 2021-06-14. (LA-UR-21-24330)

Hazarika, S., A. Biswas, E. C. Lawrence and P. J. J. Wolfram. Probabilistic Principal Component Analysis Guided Spatial Partitioning of Multivariate Ocean Biogeochemistry Data. Presented at *Visualization in Environmental Sciences 2021 workshop, co-located with EuroVis 2021 (VIRTUAL)*, zurich, Switzerland, 2021-06-14 - 2021-06-14. (LA-UR-21-24332)

Hazarika, S., A. Biswas, P. J. J. Wolfram, E. C. Lawrence and N. M. Urban. Relationship-aware Multivariate Sampling Strategy for Scientific Simulation Data. Presented at *IEEE*

Visualization 2020, Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25. (LA-UR-20-27080)

Hazarika, S., A. Biswas, P. J. J. Wolfram, E. C. Lawrence and N. M. Urban. Relationship-aware Multivariate Sampling Strategy for Scientific Simulation Data. Presented at *IEEE Visualization 2020*, Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25. (LA-UR-20-27078)

Jordanova, V. K. Key Aspects of Self-Consistent Ring Current Modeling. . (LA-UR-20-25791)

Jordanova, V. K. Inner Magnetosphere Plasma and Field Dynamics. Presented at *PWING-ERG Online Conference and School*, Nagoya, Japan, 2021-03-08 - 2021-03-12. (LA-UR-21-20090)

Klein, N. E. Statistical analysis of topologically-tracked fast flows. Presented at *IEEE Visualization 2021*, Online, New Mexico, United States, 2021-10-24 - 2021-10-24. (LA-UR-21-30493)

Klein, N. E., D. Banesh, S. K. Morley, V. K. Jordanova, M. G. Henderson and E. C. Lawrence. Identification and analysis of earthward fast flows in space weather simulations. Presented at *2nd Eddy Cross Disciplinary Symposium*, Online, New Mexico, United States, 2021-06-07 - 2021-06-10. (LA-UR-21-24933)

Klein, N. E., Y. Wang, A. L. Lui, M. F. Dorn and E. C. Lawrence. In Situ Uncertainty Quantification. Presented at *Joint Statistical Meetings*, Online, New Mexico, United States, 2021-08-08 - 2021-08-12. (LA-UR-21-26621)

Lawrence, E. C. Computer Experiments at Los Alamos National Laboratory: Life on Mars and Really Big Computers. Presented at *The University of Michigan Department of Statistics Distinguished Alumni Speaker Series*, Ann Arbor, Michigan, United States, 2020-02-14 - 2020-02-14. (LA-UR-20-21574)

Lawrence, E. C. In Situ Uncertainty Quantification for Exascale. Presented at *Verification, Validation, and Uncertainty Quantification Across Disciplines*, Chicago, Illinois, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-24589)

Lawrence, E. C., A. Biswas, L. Van Roekel, S. Dutta, L. Tang, S. K. Morley, N. E. Klein, S. Hazarika, M. J. Grosskopf, N. Panda, M. F. Dorn, K. N. Rumsey and D. Banesh. In Situ Inference Project Appraisal. Presented at *In Situ Inference Project Appraisal*, Los Alamos, New Mexico, United States, 2020-12-22 - 2020-12-22. (LA-UR-20-30332)

Moran, K. R. Advances in Bayesian Factor Modeling and Scalable Gaussian Process Regression. Presented at *2021 World Meeting of the International Society for Bayesian Analysis*, Virtual, New Mexico, United States, 2021-06-28 - 2021-07-02. (LA-UR-21-26009)

Morley, S. K. Application Domain Background. Presented at *VIS2021*, Online, New Mexico, United States, 2021-10-27 - 2021-10-27. (LA-UR-21-30666)

Morley, S. K., D. Banesh, N. E. Klein, S. Hazarika, V. K. Jordanova, M. G. Henderson, E. C. Lawrence and A. Biswas. Objective

and scalable feature identification and analysis in high-resolution simulations: Application to bursty bulk flows. Presented at *American Geophysical Union (AGU) Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32172)

W. Myren, S. T. In-situ Inference for Exascale Computing. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-04 - 2020-08-04. (LA-UR-20-25683)

Shen, J., A. Biswas and E. C. Lawrence. Sampling with Sparse Gaussian Process for Fast In-situ Inference. . (LA-UR-21-27794)

Shen, J., S. K. Morley and A. Biswas. Data reduction for large-scale space weather models using machine learning. . (LA-UR-20-26376)

Tang, L., S. Dutta and N. E. Klein. In-Situ Data Analysis with Julia for E3SM at Large Scale. Presented at *JuliaCon 2021*, Los Alamos (Virtual), New Mexico, United States, 2021-07-28 - 2021-07-30. (LA-UR-21-26078)

Urban, N. M., A. Biswas, E. C. Lawrence, M. F. Dorn, S. Dutta, M. J. Grosskopf, S. Hazarika, M. G. Henderson, V. K. Jordanova, S. K. Morley, S. T. W. Myren, D. A. Oyen, L. Tang, L. Van Roekel and J. D. Wolfe. In-Situ Inference: Bringing advanced data science into exascale simulations. . (LA-UR-20-23505)

Wang, Y., N. E. Klein, S. K. Morley, V. K. Jordanova, M. G. Henderson, A. Biswas and E. C. Lawrence. TributaryPCA: Distributed Streaming PCA for Exascale Scientific Simulations. Presented at *The 7th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-7)*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14. (LA-UR-21-30416)

Wang, Y., N. E. Klein and E. C. Lawrence. Streaming Distributed PCA for Climate Modeling. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27302)

Vander Wiel, S. A. and E. C. Lawrence. Comments on – Gibbs for Polytopes & – Multinomial Dempster-Shafer. Presented at *2021 Joint Statistical Meetings*, Online, New Mexico, United States, 2021-08-08 - 2021-08-12. (LA-UR-21-27460)

Posters

Banesh, D., R. R. Linn and J. M. Patchett. SciVis Contest 2022: Vorticity-driven Lateral Spread Ensemble Data Set. Presented at *IEEE Vis 2021*, Los Alamos, New Mexico, United States, 2021-10-24 - 2021-10-24. (LA-UR-21-29101)

Hazarika, S. Neural Network Assisted Visual Analysis. Presented at *Los Alamos - Arizona Days Conference 2021 (Virtual)*, Los Alamos, New Mexico, United States, 2021-05-17 - 2021-05-18. (LA-UR-21-24594)

Hazarika, S., L. Tang, S. K. Morley, V. K. Jordanova, M. G. Henderson, A. Biswas and E. C. Lawrence. Unsupervised Clustering and In situ Feature Tracking in Magnetospheric Simulation. Presented at *2nd Eddy Cross Disciplinary*

Symposium, Virtual, New Mexico, United States,
2021-06-07 - 2021-06-10. (LA-UR-21-24747)

Uncertainty Quantification for Robust Machine Learning

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Project Description

This project will develop uncertainty quantification tools needed to verify and validate artificial intelligence models for high stakes scientific applications. Assurance is one of the most challenging problems facing artificial intelligence (AI). Assurance addresses the question of whether an AI model has been constructed, trained, and deployed so that it is appropriate for its intended use. Building such assured AI models for science problems is complex because science is evolutionary where scientists often recycle past data and models. Training machine learning models on data produced by simulations invariably omits both the complexities and the subtle statistical patterns of real-world science datasets. This project will advance our understanding of quantifying uncertainty in machine learning (ML) and developing the needed software tools to apply ML to the challenges of mission-critical science and security problems.

Publications

Journal Articles

*Castorena, J., D. Oyen, A. Ollila, C. Legget and N. Lanza. Deep spectral CNN for laser induced breakdown spectroscopy. 2021. *Spectrochimica Acta Part B: Atomic Spectroscopy*. **178**: 106125. (LA-UR-20-28315 DOI: 10.1016/j.sab.2021.106125)

Chen, Y., Y. T. Lin, E. F. Miller, J. Neumann, A. Mallela, R. G. Posner and W. S. Hlavacek. Impacts of vaccination and SARS-CoV-2 variants on COVID-19 transmission dynamics. Submitted to *Emerging Infectious Diseases*. (LA-UR-21-30374)

Eren, M. E., J. S. Moore, E. W. Skau, E. A. Moore, M. Bhattarai, G. Chennupati and B. Alexandrov. General-Purpose Unsupervised Cyber Anomaly Detection via Non-Negative Tensor Factorization. Submitted to *ACM Digital Threats: Research and Practice (DTRAP)*. (LA-UR-22-21176)

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

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

Lin, Y. T. and N. E. Buchler. Gene expression noise accelerates the evolution of a biological oscillator. Submitted to *iScience*. (LA-UR-21-32251)

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

Neumann, J., Y. T. Lin, A. Mallela, E. F. Miller, J. Colvin, A. T. Duprat, Y. Chen, W. S. Hlavacek and R. G. Posner. Implementation of a practical Markov chain Monte Carlo sampling algorithm in PyBioNetFit. Submitted to *Bioinformatics*. (LA-UR-21-29283)

Conference Papers

Garcia Cardona, C., Y. T. Lin and T. Bhattacharya. UNCERTAINTY QUANTIFICATION FOR DEEP LEARNING REGRESSION MODELS IN THE LOW DATA LIMIT. Presented at *Uncertainty Quantification in Computational Sciences and Engineering*. (Athens, Greece, 2021-06-27 - 2021-06-30). (LA-UR-21-22482)

Castorena, J. E. and D. A. Oyen. Learning to pre-process Laser Induced Breakdown Spectroscopy Signals without clean data. Presented at *IEEE International Conference on Acoustics, Signals and Systems 2022*. (Singapore, Singapore, 2022-05-22 - 2022-05-27). (LA-UR-21-29860)

Klein, N. E., N. Panda, P. J. Gasda and D. A. Oyen. Structured Normalizing Flow Gaussian Processes for Generative Modeling of Spectroscopic Data. Presented at *1st Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI2ASE)*. (Vancouver, Canada, 2022-02-28 - 2022-02-28). (LA-UR-21-31245)

Kontolati, K., N. E. Klein and N. Panda. Neural Density Estimation and Uncertainty Quantification for Laser Induced Breakdown Spectroscopy Spectra. Presented at *Machine Learning and the Physical Sciences Workshop at the 35th Conference on Neural Information Processing Systems (NeurIPS)*. (Online, New Mexico, United States, 2021-12-13 - 2021-12-14). (LA-UR-21-27763)

Kucer, M., D. A. Oyen and G. Kenyon. Supplemental materials: On visual self-supervision and its effect on model robustness. Presented at *CVPR 2022*. (New Orleans, Louisiana, United States, 2022-06-19 - 2022-06-24). (LA-UR-21-32039)

Kucer, M., D. A. Oyen and G. Kenyon. Supplementary materials: When does visual self-supervision aid adversarial training in improving robustness to adversarial perturbations?. Presented at *Thirty-ninth International Conference on Machine Learning*. (Baltimore, Massachusetts, United States, 2022-07-17 - 2022-07-23). (LA-UR-22-20731)

Kucer, M., D. A. Oyen and G. Kenyon. When does visual self-supervision aid adversarial training in improving robustness to adversarial perturbations?. Presented at *The Thirty-ninth International Conference on Machine Learning*. (Baltimore, Massachusetts, United States, 2022-07-17 - 2022-07-23). (LA-UR-22-20763)

Kucer, M. and D. A. Oyen. On visual self-supervision and its effect on model robustness.. Presented at *CVPR 2022*. (New Orleans, Louisiana, United States, 2022-06-19 - 2022-06-24). (LA-UR-21-31340)

Ma, Y. J., J. S. Moore, G. Pleiss, D. Jayaraman and J. R. Gardner. What Matters More and When: Epistemic or Aleatoric Uncertainty?. Presented at *Neural Information Systems Processing (NeurIPS) 2021*. (Virtual-only, New Mexico, United States, 2021-12-06 - 2021-12-14). (LA-UR-21-25561)

Maus, N., H. T. Jones, J. S. Moore, M. J. Kusner, J. Bradshaw and J. R. Gardner. Local Latent Space Bayesian Optimization over Structured Inputs. Presented at *International Conference on Machine Learning (ICML 2022)*. (Baltimore, Maryland, United States, 2022-07-17 - 2022-07-23). (LA-UR-22-20779)

Moore, J. S. and H. T. Jones. Is the Discrete VAE's Power Stuck in its Prior?. Presented at *1st I Can't Believe It's Not Better Workshop (ICBINB@NeurIPS 2020)*. (Vancouber, Canada, 2020-12-12 - 2020-12-12). (LA-UR-20-29898)

Oyen, D. A., M. L. Dubey and M. Kucer. Duplicate Image Detection for Fast Identification of Easily-Confused Classes in ImageNet. Presented at *NeurIPS Workshop on ImageNet*. (Virtual, New Mexico, United States, 2021-12-13 - 2021-12-13). (LA-UR-21-29269)

Ren, C. X., A. Ziemann, J. P. Theiler and J. S. Moore. Deepfaking-it: experiments in generative, adversarial multispectral remote sensing. Presented at *SPIE*. (Orlando, Florida, United States, 2021-04-12 - 2021-04-16). (LA-UR-21-23903)

Springer, J. M., M. Mitchell and G. Kenyon. A Little Robustness Goes a LongWay: Leveraging Universal Features for Targeted Transfer Attacks. Presented at *NIPS*. (Los Alamos, New Mexico, United States, 2021-12-04 - 2021-12-04). (LA-UR-21-25273)

Teti, M. A., J. S. Moore, G. Kenyon and B. J. Migliori. LCANets: Lateral Competition Improves Robustness Against Corruption and Attack. Presented at *International Conference on Machine Learning (ICML 2022)*. (Baltimore, Maryland, United States, 2022-07-17 - 2022-07-23). (LA-UR-22-20952)

Reports

Springer, J. M., M. Mitchell and G. Kenyon. Adversarial Perturbations Are Not So Weird: Entanglement of Robust and Non-Robust Features in Neural Network Classifiers. Unpublished report. (LA-UR-21-21945)

M. Strauss, C. S. and G. Kenyon. Transfer Learning using Denoising Auto-Encoders for Cellular-Level Annotation of Tumor in Pathology Slides. Unpublished report. (LA-UR-21-21957)

Presentation Slides

Dubey, M. L., D. A. Oyen and P. J. Gasda. Improving Oxide Estimation in ChemCam Data with Regularized Linear Regression. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27465)

Dubey, M. L., P. J. Gasda and D. A. Oyen. Random Forests on Mars: Ensemble Methods for Enhanced ChemCam Calibration. . (LA-UR-21-29930)

Dubey, M. L., P. J. Gasda and D. A. Oyen. Random Forests on Mars: Ensemble Methods for Enhanced ChemCam Calibration. Presented at *Lunar and Planetary Science Conference*, Online, Texas, United States, 2022-03-07 - 2022-03-11. (LA-UR-22-21852)

Eren, M. E., J. S. Moore, B. Alexandrov, E. W. Skau, E. A. Moore and M. Bhattarai. General-Purpose Unsupervised Cyber Anomaly Detection via Non-Negative Tensor Factorization. . (LA-UR-21-30733)

Hengartner, N. W. Estimating the epidemic growth rate and the reproductive number R0 of SARS-CoV-2. Presented at *American Physical Society annual confernece*, Virtual, New Mexico, United States, 2021-03-14 - 2021-03-19. (LA-UR-21-22646)

Hengartner, N. W. Estimation of the observable map of a dynamical systems: A statistician's venture into dynamical systems. Presented at *SIAM Dynamical systems conference*, Portland, Oregon, United States, 2021-05-24 - 2021-05-24. (LA-UR-21-25050)

Holguin, F., N. E. Klein, N. Panda, J. S. Moore and D. A. Oyen. Uncertainty Quantification using Supervised Learning for ChemCam. Presented at *LANL Applied Machine Learning summer workshop presentation*, Los Alamos, New Mexico, United States, 2021-08-11 - 2021-08-11. (LA-UR-21-27933)

Klein, N. E., N. Panda, P. J. Gasda and D. A. Oyen. Generative structured normalizing flow Gaussian processes applied to spectroscopic data. Presented at *AAAI Conference on Artificial Intelligence*, Online, Canada, 2022-02-23 - 2022-02-23. (LA-UR-22-21323)

Klein, N. E., P. J. Gasda, J. E. Castorena and D. A. Oyen. Gaussian process variational autoencoders for generative modeling of ChemCam data. Presented at *Planetary Science Informatics & Data Analytics*, Online, New Mexico, United States, 2021-06-30 - 2021-06-30. (LA-UR-21-25397)

Klein, N. E., P. J. Gasda, J. E. Castorena and D. A. Oyen. Generative Modeling of ChemCam Spectroscopy Data Using Machine Learning. Presented at *Data Science for Accelerating the Understanding of Materials Workshop*, Online, New Mexico, United States, 2021-07-27 - 2021-07-29. (LA-UR-21-27229)

Kontolati, K., N. Panda, N. E. Klein, J. S. Moore and D. A. Oyen. Neural Density Estimation and Uncertainty Quantification for ChemCam Spectra. . (LA-UR-21-28078)

Moore, J. S., M. A. Teti, H. T. Jones, J. M. Springer and G. Kenyon. What Does Robustness Tell Us About Our Models?. Presented at *AI4Opt - LANL meeting*, Los Alamos, New Mexico, United States, 2022-02-03 - 2022-02-03. (LA-UR-22-20960)

Oyen, D. A. Can we Trust Machine Learning Predictions to Answer Science Questions?. Presented at *Youngstown State University*, Youngstown, Ohio, United States, 2021-04-14 - 2021-04-14. (LA-UR-21-23709)

Rego, J. R., E. Kim and G. Kenyon. Biologically Inspired Robust Perception Approximating Sparse Coding. . (LA-UR-21-29039)

Posters

Jones, H. T. and J. S. Moore. Is the Discrete VAE's Power Stuck in its Prior?. Presented at *1st I Can't Believe It's Not Better Workshop (ICBINB@NeurIPS 2020)*, Online, New Mexico, United States, 2020-12-12 - 2020-12-12. (LA-UR-20-30005)

Klein, N. E., N. Panda, P. J. Gasda and D. A. Oyen. Generative structured normalizing flow Gaussian processes applied to spectroscopic data. Presented at *AAAI Conference on Artificial Intelligence*, Online, Canada, 2022-02-22 - 2022-02-22. (LA-UR-22-21243)

The Optimization of Machine Learning: Imposing Requirements on Artificial Intelligence

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Project Description

By advancing and synthesizing the areas of machine learning (ML), this project integrates areas of that are central to Department of Energy (DOE) and Los Alamos National Laboratory (LANL) science and mission needs. In areas as diverse as non-proliferation, materials, and complex engineered systems, emerging DOE challenges are an outcome of larger and larger volumes of complicated data, for which it is natural to suggest ML as a solution. However, DOE analyses in these areas are mission critical and have high consequences for failure, and hence require high confidence ML solutions. We identify the core information sciences problems that are directly relevant for high-consequence DOE decision making and devise novel efficient constrained machine learning algorithms with robustness and efficiency guarantees. Through a unique and strong collaboration between top optimization, machine learning, and domain scientists at LANL, we develop a novel machine learning paradigm that combines constrained optimization, robust optimization, and tractability with machine learning to meet key Information Science & Technology (IS&T) challenges. The applied value of this research is demonstrated by sharpening the solutions for problems in ground feature detection and complex engineered energy systems.

Publications

Journal Articles

Chertkov, M., V. Y. Chernyak and Y. Maximov. Gauges, Loops, and Polynomials for Partition Functions of Graphical Models. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-20-30432)

Deka, D., h. doddi, S. Misra and M. Salapaka. Tractable learning in under-excited power grids. Submitted to *IEEE Transactions on Control of Network Systems*. (LA-UR-21-29122)

K. Hari, S. K., S. Rathinam, S. Darbha, K. Kalyanam, S. G. Manyam and D. W. Casbeer. Bounds on Optimal Revisit Times in Persistent Monitoring Missions With a Distinct/Remote Service Station. Submitted to *IEEE Transactions on Robotics*. (LA-UR-21-21482)

Lukashevich, A., V. Gorchakov, P. Vorobev, D. Deka and Y. Maximov. Importance Sampling Approach to Chance-Constrained DC Optimal Power Flow. Submitted to *Elsevier EPSR*. (LA-UR-21-31757)

Lukashevich, A. and Y. Maximov. Power Grid Reliability Estimation via Adaptive Importance Sampling. Submitted to *Systems & Control Letters*. (LA-UR-21-24000)

Misra, S., K. Sundar, R. Sharma and K. Brink. Deployable, Data-Driven Unmanned Vehicle Navigation System in GPS-Denied, Feature-Deficient Environments. Submitted to *Journal of Intelligent and Robotic Systems*. (LA-UR-21-20249)

Conference Papers

Bent, R. W., B. A. Tasseff and C. J. Coffrin. INFRASTRUCTUREMODELS: Composable Multi-Infrastructure Modeling in Julia. Presented at *Power Systems Computation Conference*. (Porto, Portugal, 2022-06-27 - 2022-06-27). (LA-UR-21-29947)

Bent, R. W., C. J. Coffrin and B. A. Tasseff. Modeling Electric Power Systems and Interdependencies with Natural Gas and Water: An Optimization Software Solution. Presented at *Power Systems Computation Conference*. (Porto, Portugal, 2022-06-27 - 2022-06-27). (LA-UR-21-29852)

Burashnikova, A., Y. Maximov, M. Clausel, C. Laclau, F. Iutzeler and M. R. Amini. Learning over No-Preferred and Preferred Sequence of Items for Robust Recommendation (Extended Abstract). Presented at *IJCAI (International Jount Conference on Artificial Intelligence)*. (Vienna, Austria, 2022-07-01 - 2022-07-08). (LA-UR-22-22124)

Cengil, M. F., H. Nagarajan, R. W. Bent, S. Eksioglu and B. Eksioglu. Learning to Accelerate Globally Optimal Solutions to the AC Optimal Power Flow Problem. Presented at *Power Systems Computation Conference*. (Porto, Portugal, 2022-06-27 - 2022-07-01). (LA-UR-21-30785)

Hijazi, H. L. and S. Gopinath. Benchmarking Large-Scale ACOPF Solutions and Optimality Bounds. Presented at *Power & Energy Society (PES) General Meeting*. (Denver,

Colorado, United States, 2022-06-17 - 2022-06-17). (LA-UR-21-31170)

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

Reports

Amini, M. R., V. Feofanov, L. Pauletto, E. Devijver and Y. Maximov. Self-Training: A Survey. Unpublished report. (LA-UR-22-21924)

Burashnikova, A., M. Clausel, C. Laclau, F. Iutzeler, Y. Maximov and M. Amini. Learning over no-Preferred and Preferred Sequence of Items for Robust Recommendation. Unpublished report. (LA-UR-20-30431)

Burashnikova, A., M. Clausel, M. R. Amini, N. Dante and Y. Maximov. Recommender systems : when memory matters. Unpublished report. (LA-UR-21-31786)

Lokhov, A. and M. D. Vuffray. Advanced AI solutions for locating forced oscillations in critical infrastructures. Unpublished report. (LA-UR-21-32165)

Lukashevich, A. and Y. Maximov. Power Grid Reliability Estimation via Adaptive Importance Sampling. Unpublished report. (LA-UR-21-22685)

Mitrovic, M., D. Deka, P. Vorobev and Y. Maximov. Data-Driven Stochastic AC-OPF using Gaussian Processes. Unpublished report. (LA-UR-22-21807)

Sidana, S., M. Trofimov, O. Horodnitskii, C. Laclau, Y. Maximov and M. R. Amini. User Preference and Embedding Learning with Implicit Feedback for Recommender Systems. Unpublished report. (LA-UR-20-30410)

Presentation Slides

Coffrin, C. J. A Brief Introduction to Mathematical Optimization in Julia (Part 1). Presented at *2021 Grid Science Winter School & Conference*, Los Almos, New Mexico, United States, 2021-01-11 - 2021-01-15. (LA-UR-21-20278)

Fox, Z. R., Y. T. Lin and A. V. Zlotnik. Graph interface learning for paired point clouds to identify biological binders. Presented at *AI4Opt Institute Meeting*, Los Alamos, New Mexico, United States, 2022-02-03 - 2022-02-03. (LA-UR-22-20569)

Lokhov, A. Physics-Inspired Machine Learning and Data Analytics for Energy Systems. . (LA-UR-21-22541)

Lokhov, A. Real-time Anomaly Detection and Classification in Streaming PMU Data. Presented at *PowerTech 2021*, Madrid, Spain, 2021-06-28 - 2021-06-28. (LA-UR-21-26132)

Schultz-Fellenz, E. S. Applied ML Needs in Uncrewed Aerial Systems. . (LA-UR-22-21378)

Tasseff, B. A. Optimization of Critical Infrastructure with Fluids. . (LA-UR-21-26827)

Other

Collins, A. D. and H. L. Hijazi. TA-51 PJ Site LIDAR 2020_09_18_18_45_45. Dataset. (LA-UR-20-28094)

Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems

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Project Description

This work seeks to develop new, more accurate, atomic models for the behavior of aged materials for the purpose of Stockpile Stewardship. Significantly, the ability of these newly developed interatomic potentials to track additional physical variables will give new insights into the behavior of these materials under extreme conditions, where experiments are either difficult or impossible to perform. Further, the incorporation of experimental data, obtained through purpose-built experiments, will produce models of unprecedented accuracy. The active learning framework will also seek to develop potentials for carbon based systems, such as polymers and ionic liquids. Critically, these new potentials will have the ability to track additional physical variables which will make them more accurate than previous potentials and capable of capturing new physical phenomena. Due to the huge diversity in carbon based molecules, these potentials will provide new methods for rapidly simulating many possible molecular systems and accelerating the discovery of new materials for additive manufacture. Additionally, these potentials can model the behavior of conventional explosives, an area critical to Los Alamos National Laboratory missions.

Publications

Journal Articles

Kulichenko, M., J. S. Smith, B. T. Nebgen, N. S. Fedik, N. E. Lubbers, Y. W. Li, K. M. Barros, A. I. Boldyrev and S. Tretiak. The rise of data science for materials and chemical dynamics. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-23254)

Li, T., Y. Wang, W. Li, D. Mao, C. J. Benmore, H. Xing, Q. Li, F. Wang, G. Sivaraman, A. Janotti, S. Law and T. Gu. Structure phase transition in layered materials for integrated photonic memory. Submitted to *Nature Photonics*. (LA-UR-21-30387)

*Magedov, S., C. Koh, W. Malone, N. Lubbers and B. Nebgen. Bond order predictions using deep neural networks. 2021. *Journal of Applied Physics*. **129** (6): 064701. (LA-UR-21-30590 DOI: 10.1063/5.0016011)

Sifain, A. E., L. A. Lystrom, R. A. Messerly, J. S. Smith, B. T. Nebgen, K. M. Barros, S. Tretiak, N. E. Lubbers and B. J. Gifford. Predicting Phosphorescence and Inferring Wavefunction Localization with Machine Learning. Submitted to *Chemical Science*. (LA-UR-21-21632)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, H. A. Nam, T. C. Germann, S. J. Fensin and K. M. Barros. Automated discovery of a robust interatomic potential for aluminum. Submitted to *Nature Communications*. (LA-UR-20-22194)

Tretiak, S., R. Zubatyuk, M. Kulichenko, N. E. Lubbers, J. S. Smith, B. T. Nebgen, R. A. Messerly, Y. W. Li, A. I. Boldyrev, O. Isayev and N. S. Fedik. Machine Learning for Molecular Properties: Going Beyond Interatomic Potentials. Submitted to *Nature Reviews Chemistry*. (LA-UR-21-29272)

Zhou, G., N. E. Lubbers, K. M. Barros, B. T. Nebgen and S. Tretiak. Machine Learning with Domain Knowledge in Quantum Chemistry: Learning Dynamically Responsive Semi-Empirical Quantum Mechanics.. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-30735)

*N. B. *. L. N. *. S. J. S. *. Z. R. *. Z. G. *. K. C. *. B. K. *. I. O. *. T. S. Zubatiuk, T. *., J. S. Smith, S. Tretiak, B. Nebgen, N. Lubbers, C. Koh and K. Barros. Machine learned H \xc3\xbcckel theory: Interfacing physics and deep neural networks. 2021. *The Journal of Chemical Physics*. **154** (24): 244108. (LA-UR-21-30589 DOI: 10.1063/5.0052857)

*S. J. S. *. N. B. T. *. T. S. *. I. O. Zubatyuk, R. *., J. S. Smith, B. T. Nebgen and S. Tretiak. Teaching a neural network to attach and detach electrons from molecules. 2021. *Nature Communications*. **12** (1): 4870. (LA-UR-21-30591 DOI: 10.1038/s41467-021-24904-0)

Reports

Angermeier, W., C. Barros, I. D. Dumitru, M. C. Holmes, J. R. Howard, S. R. Johnstun, G. B. King, J. T. Lindbloom, N. P.

Lordi, A. Luu, S. E. Martinez, J. N. McBride, E. S. Nelluvelil, K. T. O'Dell, H. R. Pace, N. A. Poole, A. Ramkumar, S. M. Riedel, L. Singh, S. R. Venkat, D. A. Weatherred, J. Y. Wei, K. A. York, F. Yousuf, M. T. Andrews, D. M. Israel and J. A. Kulesza. Final Reports of the 2021 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-21-28941)

Kozlowski, P. M., D. Montgomery, E. N. Loomis, T. J. Murphy, B. T. Nebgen and B. Nagler. Investigation of density and ionization dependent shifts in low charge state fluorescence of warm dense iron. Unpublished report. (LA-UR-20-28998)

Presentation Slides

Barros, K. M. Using machine learning to build robust interatomic potentials for bulk metals. Presented at *Machine Learning in Chemical and Materials Sciences*, Los Alamos, New Mexico, United States, 2021-05-13 - 2021-05-13. (LA-UR-21-24661)

Dahlbom, D. A., K. M. Barros and Y. W. Li. Fast Langevin Spin Dynamics on Many GPUs. . (LA-UR-21-27534)

Howard, J. R., A. Ramkumar, B. T. Nebgen and J. S. Smith. History dependent interatomic potentials for non-equilibrium materials. Presented at *Computational Physics Workshop Final Presentation*, Los Alamos, New Mexico, United States, 2021-08-10 - 2021-08-10. (LA-UR-21-28092)

Li, Y. W. Machine learning-assisted studies of material properties. Presented at *Brazilian Meeting on Statistical Physics*, Virtual, Brazil, 2021-11-22 - 2021-11-25. (LA-UR-21-31690)

Lubbers, N. E. Physics-informed neural networks for atomistic simulation. Presented at *The 34th annual CSP Workshop*, Athens, Georgia, United States, 2021-02-22 - 2021-02-25. (LA-UR-21-21905)

Lubbers, N. E. Adapting Neural Networks to Atomistic Systems for End-to-End Learning. Presented at *SIAM Conference on Computational Science and Engineering (CSE21)*, Fort Worth, Texas, United States, 2021-03-01 - 2021-03-05. (LA-UR-21-22108)

Lubbers, N. E. Bridging Computational Scales with Machine Learning. . (LA-UR-21-23836)

Makos, M. Z., R. B. Jadrich, E. Kraka, K. M. Barros, N. E. Lubbers and J. S. Smith. ML-based nano-reactor potential via active learning. Presented at *PASC21 Conference*, Geneva, Switzerland, 2021-07-05 - 2021-07-09. (LA-UR-21-26201)

Nebgen, B. T. My path to becoming a DOE scientist. . (LA-UR-22-21251)

Nebgen, B. T. Midterm Report: Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems. . (LA-UR-22-21833)

Nebgen, B. T. Interfacing experimental data with machine learned interatomic potentials. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22435)

Nebgen, B. T., J. S. Smith, S. Tretiak and N. E. Lubbers. Closeout Report: Machine Learned Effective Hamiltonians for Molecular Properties. . (LA-UR-21-21990)

Smith, J. S. Robust atomistic potentials from machine learning. . (LA-UR-21-23605)

Tretiak, S. Coherent PhotoexcitedDynamics and Intermolecular Conical Intersections. . (LA-UR-20-29261)

Tretiak, S. Coherent PhotoexcitedDynamics and Intermolecular Conical Intersections. Presented at *Materials research Society*, Boston, Massachusetts, United States, 2020-11-30 - 2020-11-30. (LA-UR-20-29260)

Tretiak, S. Coherent PhotoexcitedDynamics and Intermolecular Conical Intersections. Presented at *Quantum Dynamics of Excitonsand Exciton-Light Interactions*, Virtual, New Mexico, United States, 2021-03-19 - 2021-03-19. (LA-UR-21-22230)

Tretiak, S. Photoexcited dynamics in molecular materials with Non-adiabatic EXcited state Molecular Dynamics (NEXMD) code. Presented at *CyberTraining Workshop, Buffalo University*, Buffalo, New York, United States, 2021-06-18 - 2021-06-18. (LA-UR-21-25729)

Tretiak, S. Machine Learning for materials and chemical dynamics. Presented at *Data-driven physical simulation (DDPS) seminars LLNL, CA*, Livermore, California, United States, 2022-02-11 - 2022-02-11. (LA-UR-22-21193)

Zhou, G., N. E. Lubbers, K. M. Barros, B. T. Nebgen and S. Tretiak. Machine Learning with Domain Knowledge in Quantum Chemistry. Presented at *Telluride Workshop "Machine Learning and Informatics for Chemistry and Materials"*, Telluride, Colorado, United States, 2021-09-27 - 2021-10-01. (LA-UR-21-29365)

Posters

Philip, A. M., G. Zhou and B. T. Nebgen. Transition Path Search For Light-Driven Molecular Motor. . (LA-UR-21-32409)

Other

Magedov, S. I., C. F. Koh, W. F. I. Malone, N. E. Lubbers and B. T. Nebgen. Dataset of Bond Orders for Organic Molecules. Dataset. (LA-UR-20-30152)

Nebgen, B. T. Dataset of Molecular Orbital Energies and Densities for Organic Molecules. Dataset. (LA-UR-21-23368)

Nebgen, B. T., J. S. Smith, N. E. Lubbers, K. M. Barros and S. Tretiak. Dataset of energies and forces on tin configurations for machine learned interatomic potentials. Dataset. (LA-UR-21-31241)

Sifain, A. E., L. A. Lystrom, R. A. Messerly, J. S. Smith, B. T. Nebgen, K. M. Barros, S. Tretiak, N. E. Lubbers and B. J. Gifford. Dataset of Singlet and Triplet Energies and Forces for Organic Molecules. Dataset. (LA-UR-21-25454)

Machine Learning for Realizing Next-Generation Quantum Hardware

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Project Description

Quantum technologies (QT) are today poised to revolutionize computing and sensing, with applications in fundamental science and national security. However, as quantum systems grow in size and complexity, controlling QT while preserving and optimally exploiting fragile quantum correlations becomes intractable using standard, human-directed approaches. Our ability to harness quantum effects limits the quantum advantage of a given system, be it a sensor or quantum computer. We address this challenge by integrating machine learning (ML; a powerful new set of tools for working with complex data and systems), with quantum hardware developed at Los Alamos National Laboratory to create a new generation of QT. With this approach, we discover new approaches to (1) realizing experiments with enhanced performance and robustness against environmental fluctuations, (2) generating and utilizing entangled states for optimal quantum sensing, and (3) error mitigation in quantum computing/ simulation. Further, we note that this work impacts ML by incorporating physics domain knowledge into ML approaches, leveraging uncertainty quantification techniques to produce optimally robust models, and by demonstrating reproducibility in ML-based models. These are cutting-edge topics in the scientific ML community. Thus, with this synthesis of ML and QT, we advance the state of the art in ML and QT.

Publications

Journal Articles

Amico, L., D. Anderson, M. G. Boshier, J. Brantut, L. C. Kwek, A. Minguzzi and W. von Klitzing. Atomtronic circuits: from basic research in many-body physics to applications for quantum technologies. Submitted to *Reviews of Modern Physics*. (LA-UR-21-27329)

Caro, M., L. Cincio, J. Gibbs, Z. P. Holmes, N. A. Ezzell, H. Huang, A. T. Sornborger and P. J. Coles. Dynamical simulation via quantum machine learning with provable generalization. Submitted to *PRL*. (LA-UR-22-20965)

Cincio, L., D. Bultrini, M. E. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith and P. J. Coles. Unifying and benchmarking state-of-the-art quantum error mitigation techniques. Submitted to *Quantum*. (LA-UR-21-27288)

Czarnik, P. J., A. T. Arrasmith, L. Cincio and P. J. Coles. Qubit-efficient exponential suppression of errors. Submitted to *arXiv+PRX Quantum*. (LA-UR-21-21151)

Diaw, A., M. McKerns, I. Sagert, L. G. Stanton and M. S. Murillo. Efficient Learning of Accurate Surrogates for Simulations of Complex Systems. Submitted to *Nature Machine Intelligence*. (LA-UR-20-24947)

LaRose, R., A. Mari, S. Kaiser, P. J. Kralekas, A. A. Alves, P. J. Czarnik, M. El Mandouh, M. H. Gordon, Y. Hindy, A. Robertson, P. Thakre, N. Shammah and W. J. Zeng. Mitiq: A software package for error mitigation on noisy quantum computers. Submitted to *arXiv*. (LA-UR-21-25925)

Larocca, M., P. J. Czarnik, K. Sharma, G. Muraleedharan, P. J. Coles and M. V. S. Cerezo de la Roca. Diagnosing barren plateaus with tools from quantum optimal control. Submitted to *Physical Review X Quantum*. (LA-UR-21-24973)

*Lowe, A., M. H. Gordon, P. Czarnik, A. Arrasmith, P. J. Coles and L. Cincio. Unified approach to data-driven quantum error mitigation. 2021. *Physical Review Research*. **3** (3): 033098. (LA-UR-20-28845 DOI: 10.1103/ PhysRevResearch.3.033098)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio and P. J. Coles. Variational Quantum Algorithms. Submitted to *Nature Reviews Physics*. (LA-UR-20-30142)

S. Cerezo de la Roca, M. V., G. verdon, H. Huang, L. Cincio and P. J. Coles. Quantum Machine Learning: Challenges and Opportunities. Submitted to *Nature Computational Science*. (LA-UR-21-31504)

Volkoff, T. J. and M. J. Martin. Asymptotic optimality of twist-untwist protocols for Heisenberg scaling in atom-based sensing. Submitted to *Physical Review Research*. (LA-UR-21-23486)

Volkoff, T. J. and M. J. Martin. Asymptotic optimality of twist-untwist protocols for Heisenberg scaling in atom-based

sensing. Submitted to *Physical Review Research*. (LA-UR-21-23486)

Wang, S., P. J. Coles, P. J. Czarnik, A. T. Arrasmith, M. V. S. Cerezo de la Roca and L. Cincio. Can Error Mitigation Improve Trainability of Noisy Variational Quantum Algorithms?. Submitted to *Physical Review X, arxiv.org*. (LA-UR-21-28574)

Reports

Cincio, L. Error mitigation with Clifford quantum-circuit data. Unpublished report. (LA-UR-22-21698)

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Unpublished report. (LA-UR-21-24972)

Suau, A., J. A. Nelson, M. D. Vuffray, A. Lokhov, L. Cincio and C. J. Coffrin. Single-Qubit Cross Platform Comparison of Quantum Computing Hardware. Unpublished report. (LA-UR-21-28409)

Presentation Slides

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Czarnik, P. J. dvanced techniques for improving error mitigation. . (LA-UR-22-20301)

Czarnik, P. J., A. Lowe, M. H. Gordon, A. T. Arrasmith, P. J. Coles and L. Cincio. Data-driven error mitigation for near-term quantum computers. Presented at *Seminar of Institute of Theoretical Physics of Jagiellonian University, Cracow*, Cracow, Poland, 2020-12-10 - 2020-12-10. (LA-UR-20-30043)

Czarnik, P. J., A. Lowe, M. H. Gordon, A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation for gate-based quantum computers. Presented at *IonQ seminar*, College Park, Maryland, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-22055)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *Quantum Information Processing*, Munich, Germany, 2021-02-01 - 2021-02-05. (LA-UR-21-20721)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *APS March Meeting*, virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22444)

Krzyzanowska, K. A. Atomtronic circuits with optical dipole potentials. Presented at *Atomtronics@AbuDhabi2021*, AbuDhabi, United Arab Emirates, 2021-05-31 - 2021-06-11. (LA-UR-21-27040)

Lowe, A., M. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, P. J. Coles and L. Cincio. Unified Approach to Data Driven Quantum Error Mitigation. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22591)

Martin, M. J. Quantum information science with Rydberg atoms. . (LA-UR-20-29116)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *UNM CQuIC seminar*, Albuquerque, New Mexico, United States, 2021-02-04 - 2021-02-04. (LA-UR-21-20920)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *LANL/TAMU Quantum Seminar Series*, College Station, Texas, United States, 2021-04-27 - 2021-04-27. (LA-UR-21-23972)

Martin, M. J. Quantum information science and sensing with ultracold neutral atoms. . (LA-UR-21-25997)

Martin, M. J. Quantum information science with laser-dressed atoms Q-SEnSE Convergence Seminar. Presented at *Q-SEnSE Convergence Seminar*, Boulder, Colorado, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32107)

Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

McKerns, M. mystic: physics-informed learning and automated design/control under uncertainty. Presented at *Applied Machine Learning Symposium*, Los Alamos, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-27369)

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Presented at *CAMERA Workshop on Autonomous Discovery in Science and Engineering*, Berkeley, California, United States, 2021-04-20 - 2021-04-22. (LA-UR-21-30257)

Probst, M. J. A New Approach to Stabilizing Lasers. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27581)

S. Cerezo de la Roca, M. V. Noise, Error Mitigation, and the Trainability of the Trainability of Variational Quantum AlgorithmsVariational Quantum Algorithms. Presented at *Cuantos 3*, La Plata, Argentina, 2021-11-15 - 2021-11-17. (LA-UR-21-31308)

S. Cerezo de la Roca, M. V. A birds-eye introduction to quantum computing.. Presented at *Physics Without Frontiers: Quantum Machine Learning*, Guatemala, Guatemala, 2021-11-29 - 2021-12-03. (LA-UR-21-31310)

S. Cerezo de la Roca, M. V. Quantum Machine Learning Exercices. Presented at *PWF School on Quantum Computing*, Guatemala, Guatemala, 2021-11-29 - 2021-12-03. (LA-UR-21-31585)

Schatzki, L., E. Chitambar, G. Liu, J. Beckey and M. V. S. Cerezo de la Roca. Concentratable Entanglement and Entanglement Verification. . (LA-UR-22-20767)

Sornborger, A. T. Entanglement and Quantum Machine Learning. Presented at *Physics of Quantum Electronics*, Online, New Mexico, United States, 2022-01-10 - 2022-01-14. (LA-UR-22-20220)

Tiwari, V. Optimizing Beam Splitters for Matter Waves. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27582)

Volkoff, T. J. and M. J. Martin. QSC Spotlight on Progress for Twist-untwist protocols for Heisenberg scaling in atomic interferometry. . (LA-UR-21-26220)

Posters

Lowe, A., M. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, P. J. Coles and L. Cincio. Unified approach to data-driven quantum error mitigation. Presented at *Quantum Information Processing*, Online, New Mexico, United States, 2021-01-01 - 2021-01-05. (LA-UR-21-20496)

S. Cerezo de la Roca, M. V. Barren Plateaus and Trainability in Quantum Neural Networks: A perspective from the inductive biases viewpoint. Presented at *Quantum Information Processing*, Pasadena, California, United States, 2022-03-07 - 2022-03-11. (LA-UR-22-21844)

Enabling Predictive Scale-Bridging Simulations through Active Learning

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Project Description

Exascale supercomputers that will arrive in the next few years offer tremendous computational power, if one can coordinate the approximately one billion different calculations that are occurring at any given time. Our project combines these exciting advances in computing architectures with similarly exciting advances in machine learning algorithms to enable computational science and engineering simulations with greater physical fidelity, combining molecular-scale simulations with continuum fluid dynamics ones. Just as understanding nanomaterial properties has been a grand challenge over the past two decades, understanding fluids in complex nanopores is the next frontier. Our computational framework for incorporating nanoscale physics will enable efficient extraction of subsurface energy (hydrocarbon and geothermal) from tight unconventional resources which have proved to be extremely challenging. Similarly, we expect to be able to efficiently and accurately account for complex atomistic effects such as non-local transport in inertial confinement fusion (ICF) simulations, providing a valuable computational tool for understanding whether ignition is ultimately achievable and, if yes, suggest practical avenues for controlling mix, instabilities, and heat loss from the hot spot. Our active learning approach will bring about transformational advances in the way nanoconfinement effects of fluids are modeled in these and other applications.

Technical Outcomes

The team successfully executed demonstrations of active learning-enabled scale-bridging simulations for both exemplar applications, fluid flow in nanoconfined shale and inertial confinement fusion, using the common GLUE (Generic Learning User Enablement) code framework. In addition, novel machine learning techniques and applications not originally envisioned in the originally proposed work were developed and published: a reinforcement learning strategy which resulted in fast emulation of fluid flow, and thermodynamically consistent machine learning models.

Publications

Journal Articles

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

*Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. 2020. *The Journal of Chemical Physics*. **153** (10): 104502. (LA-UR-19-31421 DOI: 10.1063/5.0017894)

*Craven, G. T., N. Lubbers, K. Barros and S. Tretiak. Determination of Structural Correlation Functions. 2020. *The Journal of Physical Chemistry Letters*. **11** (11): 4372-4378. (LA-UR-19-32446 DOI: 10.1021/acs.jpclett.0c00627)

Diaw, A., K. M. Barros, J. R. Haack, C. Junghans, B. Keenan, D. Livescu, N. E. Lubbers, M. McKerns, R. S. Pavel, D. G. Rosenberger, I. Sagert, T. C. Germann and Y. W. Li. Multiscale Simulation of Plasma Flows Using Active Learning. Submitted to *Physics of Plasmas*. (LA-UR-20-23628)

Diaw, A., M. McKerns, I. Sagert, L. G. Stanton and M. S. Murillo. Efficient Learning of Accurate Surrogates for Simulations of Complex Systems. Submitted to *Nature Machine Intelligence*. (LA-UR-20-24947)

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

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

*Li, Y. W., M. Lupo Pasini, J. Yin and M. Eisenbach. A scalable algorithm for the optimization of neural network

architectures. 2021. *Parallel Computing*. 102788. (LA-UR-21-20936 DOI: 10.1016/j.parco.2021.102788)

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

*Mansi, M., M. Mehana, M. Fahes and H. Viswanathan. Thermodynamic modeling of the temperature impact on low-salinity waterflooding performance in sandstones. 2020. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. **586**: 124207. (LA-UR-19-28076 DOI: 10.1016/j.colsurfa.2019.124207)

S. Mehana, M. Z., Q. Kang, H. S. Viswanathan and H. Nasrabadi. Molecular modeling of subsurface phenomena related to petroleum engineering. Submitted to *Earth Science Reviews*. (LA-UR-20-20902)

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

S. Mehana, M. Z. and M. Fahes. Molecular Simulation Study of Low salinity Waterflooding Mechanisms. Submitted to *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. (LA-UR-20-20808)

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

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

*Mehana, M., S. A. Hosseini, T. A. Meckel and H. Viswanathan. Modeling CO2 plume migration using an invasion-percolation approach that includes dissolution. 2020. *Greenhouse Gases: Science and Technology*. **10** (2): 283-295. (LA-UR-19-26910 DOI: 10.1002/ghg.1976)

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

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

Pachalieva, A. A. and A. J. Wagner. Molecular dynamics lattice gas equilibrium distribution function for Lennard-Jones particles. Submitted to *Philosophical Transactions of the Royal Society A. Mathematical, Physical and Engineering Sciences*. (LA-UR-21-20022)

Pachalieva, A. A. and A. J. Wagner. Connecting lattice Boltzmann methods to physical reality by coarse-grainingMolecular Dynamics simulations. Submitted to *Physical Review Letters*. (LA-UR-21-28702)

Pachalieva, A. A. and A. Wagner. Non-Gaussian distribution of displacements for Lennard-Jones particles in equilibrium. Submitted to *Physical Review E*. (LA-UR-20-24192)

*Lupo Pasini, M., Y. W. Li, J. Yin, J. Zhang, K. Barros and M. Eisenbach. Fast and stable deep-learning predictions of material properties for solid solution alloys. 2021. *Journal of Physics: Condensed Matter*. **33** (8): 084005. (LA-UR-20-27481 DOI: 10.1088/1361-648X/abcb10)

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

*Rosenberger, D., N. Lubbers and T. C. Germann. Evaluating diffusion and the thermodynamic factor for binary ionic mixtures. 2020. *Physics of Plasmas*. **27** (10): 102705. (LA-UR-20-24058 DOI: 10.1063/5.0017788)

*Samarakoon, A. M., K. Barros, Y. W. Li, M. Eisenbach, Q. Zhang, F. Ye, V. Sharma, Z. L. Dun, H. Zhou, S. A. Grigera, C. D. Batista and D. A. Tennant. Machine-learning-assisted insight into spin ice Dy2Ti2O7. 2020. *Nature Communications*. **11** (1): 892. (LA-UR-19-30738 DOI: 10.1038/s41467-020-14660-y)

. Y. Y. *. J. H. *. P. W. *. K. Q. *. V. H. S. *. P. M. *. P. M. J. *. L. N. Santos, J. E., Q. Kang and H. S. Viswanathan. Computationally Efficient Multiscale Neural Networks Applied to Fluid Flow in Complex 3D Porous Media. 2021. *Transport in Porous Media*. **140 (1): 241-272. (LA-UR-21-20720 DOI: 10.1007/s11242-021-01617-y)

*Santos, J. E., M. Mehana, H. Wu, M. Prodanovic, Q. Kang, N. Lubbers, H. Viswanathan and M. J. Pyrcz. Modeling Nanoconfinement Effects Using Active Learning. 2020. *The Journal of Physical Chemistry C*. **124** (40): 22200-22211. (LA-UR-20-22427 DOI: 10.1021/acs.jpcc.0c07427)

Viswanathan, H. S., J. Ajo-Franklin, J. Birkholzer, Y. Guglielmi, J. D. Hyman, S. Karra, L. Pyrak-Nolte, H. Rajaram, G. Srinivasan and D. M. Tartakovsky. Coupled processes in fractured rock: recent advances and new frontiers. Submitted to *Reviews of Geophysics*. (LA-UR-21-28244)

Wang, K., Y. Chen, M. Z. S. Mehana, N. E. Lubbers, K. Bennett, Q. Kang, H. S. Viswanathan and T. C. Germann. A physics-informed and hierarchically regularized data-driven model for predicting fluid flow through porous media. Submitted to *Journal of Computational Physics*. (LA-UR-20-27444)

*Wu, H., W. Fang, Q. Kang, W. Tao and R. Qiao. Predicting Effective Diffusivity of Porous Media from Images by

Deep Learning. 2019. *Scientific Reports*. **9** (1): 20387. (LA-UR-19-23183 DOI: 10.1038/s41598-019-56309-x)

Conference Papers

S. Mehana, M. Z., J. W. Carey, G. D. J. Guthrie, J. D. Hyman, Q. Kang, S. Karra, C. W. Neil, M. R. Sweeney, H. Xu, H. S. Viswanathan and J. Santos. Discovery Science of Hydraulic Fracturing and Shale Fundamentals. Presented at *Unconventional Resources Technology Conference*. (Houston, Texas, United States, 2021-07-26 - 2021-07-28). (LA-UR-21-25369)

Reports

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Unpublished report. (LA-UR-21-24972)

Presentation Slides

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

Haack, J. R. Towards Enabling Predictive Scale-Bridging Simulations through Active Learning. . (LA-UR-20-23366)

Haack, J. R. Scale Bridging through Active Learning. . (LA-UR-21-20131)

Junghans, C. Novel Approaches to Multi-Scale Modeling. . (LA-UR-21-22275)

Li, Y. W. Machine Learning Assisted Monte Carlo Methods for the Studies of Materials Properties. Presented at *XXXI IUPAP Conference on Computational Physics*, Hong Kong, China, 2019-07-28 - 2019-08-01. (LA-UR-19-27508)

Lubbers, N. E. Realizing Physical Principles in Atomistic Machine Learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-19 - 2019-02-21. (LA-UR-19-21277)

Lubbers, N. E. Machine Learning & Neural Networks Tutorial. Presented at *IMAC XXXVIII*, Houston, Texas, United States, 2020-02-10 - 2020-02-13. (LA-UR-20-21292)

Lubbers, N. E. Bridging Computational Scales with Machine Learning. . (LA-UR-21-23836)

McKerns, M. rigorous model validation and engineering design under uncertainty. Presented at *Computational Data Science Approaches for Materials Conference*, Los Alamos, New Mexico, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-32500)

McKerns, M. mystic - a brief introduction. . (LA-UR-19-22525)

McKerns, M. mystic: physics-informed learning and automated design/control under uncertainty. Presented at *Applied Machine Learning Symposium*, Los Alamos, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-27369)

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Presented at *CAMERA Workshop on Autonomous Discovery in Science and Engineering*, Berkeley, California, United States, 2021-04-20 - 2021-04-22. (LA-UR-21-30257)

McKerns, M., A. Diaw, I. Sagert, L. Stanton and M. Murillo. adaptive learning with directed sampling. Presented at *Nambe Meeting*, Los Alamos, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-29586)

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

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

S. Mehana, M. Z. Data-driven Models of Adsorption Equilibria of Multi-component Mixtures in Porous Materials. Presented at *ISTI review*, Los alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-29091)

Pachalieva, A. A. Learning Lattice Boltzmann Methods via H-functions. Presented at *CNLS Postdoc Seminar*, Los Alamos, New Mexico, United States, 2020-10-01 - 2020-10-01. (LA-UR-20-27736)

Pachalieva, A. A. Deriving LBM Collision Operator using the Coarse-Graining MDLG Approach. Presented at *30th International Conference on Discrete Simulation of Fluid Dynamics (DSFD 2021)*, Viterbo, Italy, 2021-09-13 - 2021-09-17. (LA-UR-21-28925)

Pachalieva, A. A. Incorporating nanoconfinement effects into Lattice Boltzmann Method using Machine Learning and Molecular Dynamics. Presented at *Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET) 2021*, San Diego, California, United States, 2021-09-26 - 2021-09-29. (LA-UR-21-29528)

Pachalieva, A. A. and A. Wagner. Deriving LBM collision operator using the Coarse-Graining MDLG Approach. Presented at *29th International Conference on Discrete Simulation of Fluid Dynamics (DSFD 2020)*, Viterbo, Italy, 2020-07-13 - 2020-07-17. (LA-UR-20-25144)

Pavel, R. S., C. Junghans and T. C. Germann. Workflow Requirements for Active Learning Enabled Scale-Bridging Simulations. . (LA-UR-21-20939)

Rosenberger, D. G. Learning diffusion coefficients of particles with the help of thermodynamics. Presented at *2019 ALCF Simulation, Data, and Learning Workshop*, Argonne, Illinois, United States, 2019-10-01 - 2019-10-03. (LA-UR-19-29611)

Rosenberger, D. G. Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures. Presented at *APS March Meeting 2020*, Denver,

Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21573)

Rosenberger, D. G. Using machine learning to estimate ideal/non ideal mixing in binary ionic mixtures.. . (LA-UR-21-21248)

Rosenberger, D. G., N. E. Lubbers and T. C. Germann. Evaluating diffusion and the thermodynamic factor for binary ionic mixtures.. Presented at *Frontiers in Machine Learning for the Physical Sciences*, Virtual event, California, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28065)

Smith, C. D., B. Keenan, D. Livescu, J. R. Haack and R. S. Pavel. Collisional Plasma Shocks in a Warm Dense Matter Regime. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30931)

Viswanathan, H. S. Flow and Fracture in Microstructure Accelerated by Machine Learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-20 - 2019-02-20. (LA-UR-19-21272)

Viswanathan, H. S. Reducing the Environmental Footprint of Subsurface Energy. . (LA-UR-21-27612)

Viswanathan, H. S., J. A. Estrada Santos, N. E. Lubbers, A. A. Pachalieva, M. Z. S. Mehana, S. Karra, Q. Kang and T. C. Germann. Scale-bridging using machine learning: nano-confinement effects in porous media. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31882)

Viswanathan, H. S., J. W. Carey, J. D. Hyman, P. A. Johnson and D. O'Malley. Machine Learning and Quantum Studies for Fractured Systems. Presented at *Virtual BES PI meeting*, Los Alamos, New Mexico, United States, 2021-08-05 - 2021-08-05. (LA-UR-21-27613)

Posters

S. Mehana, M. Z., Q. Kang and H. S. Viswanathan. On the Molecular Modeling of Hydrocarbon Behavior in Shale Nano-pores. Presented at *LANL postdoc Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28695)

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

Rosenberger, D. G., N. E. Lubbers and T. C. Germann. Evaluating diffusion and the thermodynamic factor for binary ionic mixtures.. Presented at *Frontiers in Machine Learning for the Physical Sciences*, Virtual event, California, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28064)

Sagert, I., J. R. Haack, A. Diaw, C. Junghans, B. Keenan, N. E. Lubbers, M. McKerns, R. S. Pavel and D. Livescu. A 3D

Multi-Species Kinetic-Fluid Coupling Technique for HEDP Simulations. Presented at *International Conference on Numerical Simulations of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28767)

Smith, C. D., B. Keenan, D. Livescu, J. R. Haack and R. S. Pavel. Collisional Plasma Shocks in a Warm Dense Matter Regime. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30884)

Other

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

S. Mehana, M. Z. Dataset for Machine learning summer school. Dataset. (LA-UR-21-26705)

Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics (U)

Boian Alexandrov
20190020DR

Project Description

The world's data is the most valuable exponentially-growing resource. Terabyte scale datasets are generated every minute by massive computer simulations, large-scale experiments, and global surveillance systems. Analyses of these data are of crucial importance for global security and directly related to Department of Energy mission-critical research areas. Development of machine learning (ML) techniques for efficient and robust data analyses is of paramount importance to perform timely, accurate, and meaningful data interpretation. Our project addresses this need by developing a novel ML methodology and a unique high-performance computing toolbox to perform data analyses and extract meaningful and interpretable features from high-dimensional extra-large datasets. High-dimensional data are naturally organized in tensors (multi-dimensional arrays) and our methodology will focus on cutting-edge tensor-based ML methods utilizing novel techniques. We will target terabyte and petabyte scale datasets in this project but if this high-risk/high-reward research is successful, the developed high-performance computing tools will be able to address larger problems. The new methodology will be important for DOE, the National Nuclear Security Administration, National Security Agency, Nuclear Regulatory Commission, Enviornmental Protection Agency, National Institutes of Health, and other agencies, placing the Laboratory in a leadership position in the field of Big-Data Analytics.

Technical Outcomes

The technical goal of this project was to go beyond state-of-the-art Machine Learning methods and develop a Big-Data science methodology based on Non-Negative Factorization and Tensor Networks, capable of feature extraction, dimension reduction, anomaly detection, data fusion, and data mining. The team developed the necessary mathematical framework and implemented it in the software suite "SmartTensors AI Platform", which received two R&D 100 awards. SmartTensors' applicability was demonstrated through applications in more than 15 different fields.

Publications

Journal Articles

*Ahmmed, B., M. K. Mudunuru, S. Karra, S. C. James and V. V. Vesselinov. A comparative study of machine learning models for predicting the state of reactive mixing. 2021. *Journal of Computational Physics*. **432**: 110147. (LA-UR-20-21737 DOI: 10.1016/j.jcp.2021.110147)

*Ahmmed, B., S. C. James and J. Yelderman. Post-Calibration Uncertainty Analysis for Travel Times at a Naval Weapons Industrial Reserve Plant. 2020. *Water*. **12** (12): 3428. (LA-UR-19-31625 DOI: 10.3390/w12123428)

Ahmmed, B., S. Karra, V. V. Vesselinov and M. K. Mudunuru. Machine Learning to Discover Mineral Trapping Signatures due to CO2 Injection. Submitted to *International Journal of Greenhouse Gas Control*. (LA-UR-21-20069)

Ahmmed, B., V. V. Vesselinov, M. K. Mudunuru and S. Karra. Unsupervised machine learning to discover dominant attributes and hidden signatures of mineral precipitation due to CO2 sequestration. Submitted to *Journal of Contaminant Hydrology*. (LA-UR-20-22760)

*Akhter, N., G. Chennupati, K. L. Kabir, H. Djidjev and A. Shehu. Unsupervised and Supervised Learning over the Energy Landscape for Protein Decoy Selection. 2019. *Biomolecules*. **9** (10): 607. (LA-UR-19-27828 DOI: 10.3390/biom9100607)

Alexandrov, B., B. Zhu, M. L. Poeta, M. Costantini, T. Zhang, J. Shi, S. S. Sentinelli, V. Pompeo, M. Cardelli, B. Otlu, X. Hua, K. Jones, S. Brodie, J. R. Toro, M. Yeager, M. Wang, B. Hicks, L. B. Alexandrov, K. M. Brown, S. Chanock, V. M. Fazio, M. Gallucci and M. T. Landi. Intratumor heterogeneity and clonal expansion cascade in papillary renal cell carcinoma. Submitted to *Genome Biology*. (LA-UR-18-31218)

Alexandrov, B., C. A. Lopez Bautista and S. Gnanakaran. Unsupervised Machine Learning for Analysis of Coexisting Lipid Phases and Domain Growth in Biological Membranes. Submitted to *JCTC*. (LA-UR-18-29079)

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonic Polyadic Decomposition with Rank Deficient Factors. Submitted to *SIAM Journal on Mathematics of Data Science*. (LA-UR-19-29298)

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Submitted to *Numerical Linear Algebra with Applications*. (LA-UR-21-26100)

Alexandrov, B., D. F. DeSantis, P. M. D. Truong and E. W. Skau. Factorization of Binary Matrices: Rank Relations, Uniqueness and Model Selection of Boolean Decomposition. Submitted to *ACM Transactions on Information Systems*. (LA-UR-21-30686)

Alexandrov, B., E. W. Skau, V. Stanev and I. Takeuchi. Topic Analysis of Superconductivity Literature by Semantic Non-negative Matrix Factorization. Submitted to *Lecture Notes in Computer Science*. (LA-UR-21-31345)

Alexandrov, B., K. O. Rasmussen, G. Weissman, G. Bel, U. Yermiyahu, A. Ben-Gal and O. Dahan. Effects of salinity and soil heterogeneity on water, nitrate and bromide flow under agricultural fields. Submitted to *Vadose Zone Journal*. (LA-UR-19-31560)

Alexandrov, B., M. Bhattarai, N. S. Kharat, E. W. Skau, B. T. Nebgen, H. N. Djidjev, J. P. Smith and S. Rajopadhye. Distributed non-negative RESCAL with Automatic Model Selection for Exascale Data. Submitted to *IEEE Transactions on Knowledge and Data Engineering*. (LA-UR-22-21199)

Alexandrov, B., M. E. Eren, J. S. Moore, E. W. Skau, E. A. Moore, M. Bhattarai and G. Chennupati. Cyber Anomaly Detection via Non-negative Tensor Factorization. Submitted to *Journal of Digital Threats: Research and Practice*. (LA-UR-21-29195)

Alexandrov, B., M. E. Eren, M. Bhattarai, R. J. JOYCE, E. RAFF and C. NICHOLAS. Large-scale Semi-supervised Bulk Classification of Malware Families Under Extreme Class Imbalance via Hierarchical Non-Negative Matrix Factorization with Automatic Model Determination. Submitted to *ACM Transactions on Privacy and Security*. (LA-UR-21-31128)

Alexandrov, B., M. Karimi, V. Petkova, J. M. Asara, M. Griffin and A. Usheva. Aberrant cardiac energy metabolism in metabolic syndrome: insight from metabolomics and a pig model. Submitted to *Scientific Reports*. (LA-UR-19-25878)

Alexandrov, B., O. Ziegler, N. Sriram, V. Gelev and A. Usheva. The cardiac background in Metabolic Syndrome is an alarm for the vulnerable response to SARS-CoV-2 infection. Submitted to *Scientific Reports*. (LA-UR-20-30278)

Alexandrov, B., R. Vangara, I. Ashiqul, Y. Wu, M. D\xc3\xadaz-Gay, E. Bergstrom, Y. He, M. Barnes, M. Vella, S. Moody, S. Senkin, J. Wang, Y. R. Li, L. Riva, T. Zhang, A. J. Gruber, C. D. Steele, B. Otlu, A. Khandeka, A. Abbasi, L. Humphreys, N. Syulyukina, S. W. Brady, N. Pillay, J. Zhang, D. J. Adams, I. Marticorena, D. C. Wedge, M. Landi, P. Brennan, M. Stratton, S. G. Rozen and L. B. Alexandrov. Uncovering novel mutational signatures by de novo extraction with SigProfilerExtractor. Submitted to *Nature Genetics*. (LA-UR-20-30233)

Alexandrov, B., R. Vangara, K. O. Rasmussen, D. Petsev and G. Bel. Identification of 2D Anomalous Diffusion by Unsupervised Learning Combined with Green's Function Inverse Method. Submitted to *Physical Review E*. (LA-UR-19-25879)

*Carrillo-Cabada, H., E. Skau, G. Chennupati, B. Alexandrov and H. Djidjev. An Out of Memory tSVD for Big-Data Factorization. *IEEE Access*. **8**: 107749-107759. (LA-UR-20-22236 DOI: 10.1109/ACCESS.2020.3000508)

*Chennupati, G., R. Vangara, E. Skau, H. Djidjev and B. Alexandrov. Distributed non-negative matrix factorization with determination of the number of latent features. 2020. *The Journal of Supercomputing*. **76** (9): 7458-7488. (LA-UR-20-20469 DOI: 10.1007/s11227-020-03181-6)

DeSantis, D. F., B. Alexandrov and E. W. Skau. Factorizations of Binary Matrices - Rank Relations and the Uniqueness of Boolean Decompositions. Submitted to *Linear and Multilinear Algebra*. (LA-UR-20-30257)

DeSantis, D. F., P. J. J. Wolfram, B. Alexandrov and K. E. Bennett. Multi-resolution Cluster Analysis - Addressing Trust in Climate Classification. Submitted to *Theoretical and applied climatology*. (LA-UR-19-27331)

Eren, M. E., J. S. Moore, E. W. Skau, E. A. Moore, M. Bhattarai, G. Chennupati and B. Alexandrov. General-Purpose Unsupervised Cyber Anomaly Detection via Non-Negative Tensor Factorization. Submitted to *ACM Digital Threats: Research and Practice (DTRAP)*. (LA-UR-22-21176)

Karra, S., B. Ahmmed and M. K. Mudunuru. Dataset for Machine Learning Analysis of Reactive Mixing under Anisotropy and Heterogeneity. Submitted to *Data in brief, Elsevier*. (LA-UR-21-20064)

*Nebgen, B. T., R. Vangara, M. A. Hombrados Herrera, S. Kuksova and B. Alexandrov. A neural network for determination of latent dimensionality in Nonnegative Matrix Factorization. 2020. *Machine Learning: Science and Technology*. (LA-UR-20-20994 DOI: 10.1088/2632-2153/aba372)

O'Malley, D., H. N. Djidjev and B. Alexandrov. Boolean Tensor Factorization with QuantumAnnealers. Submitted to *npj Quantum Information*. (LA-UR-20-21860)

O'Malley, D., J. K. Golden and V. V. Vesselinov. Learning to regularize with a variational autoencoder for hydrologic inverse analysis. Submitted to *Water Resources Research*. (LA-UR-19-24983)

R. Pelofske, E. A., G. Hahn, D. O'Malley, H. N. Djidjev and B. Alexandrov. Boolean Hierarchical Tucker Networks on Quantum Annealers. Submitted to *Large-Scale Scientific Computations*. (LA-UR-21-22363)

R. Pelofske, E. A., G. Hahn, D. O'Malley, H. N. Djidjev and B. Alexandrov. Quantum Annealing Algorithms for Boolean Tensor Networks. Submitted to *IEEE Transactions on Emerging Topics in Computing*. (LA-UR-21-27414)

R. Pelofske, E. A., H. N. Djidjev and G. Hahn. Inferring the Dynamics of Ground-State Evolution of Quantum Annealers. Submitted to *Special Section on Parallel and Distributed Computing Techniques for Non-Von Neumann Technologies*. (LA-UR-20-27022)

Prakash, D. J., L. Denoyer, R. Vangara, J. M. Baca, F. van Swol and D. N. Petsev. Ionic Size Effects on the Properties of Charge Regulating Electric Double Layers. Submitted to *Molecular Physics*. (LA-UR-21-20082)

. S. E. *. D. D. *. A. B. Truong, D. P., B. Alexandrov, D. P. Truong, E. Skau and D. Desantis. Boolean Matrix Factorization via Nonnegative Auxiliary Optimization. *IEEE Access*. **9: 117169-117177. (LA-UR-21-25283 DOI: 10.1109/ACCESS.2021.3107189)

Truong, D. P., E. W. Skau, V. I. Valtchinov and B. Alexandrov. Determination of Latent Dimensionality in International Trade Flow. Submitted to *Machine Learning: Science and Technology*. (LA-UR-20-21947)

*Vangara, R., K. O. Rasmussen, D. N. Petsev, G. Bel and B. S. Alexandrov. Identification of anomalous diffusion sources by unsupervised learning. 2020. *Physical Review Research*. **2** (2): 023248. (LA-UR-20-23646 DOI: 10.1103/PhysRevResearch.2.023248)

Conference Papers

Alexandrov, B., E. W. Skau, V. Stanev and I. Takeuchi. Topic Analysis of Superconductivity Literature by Semantic Non-negative Matrix Factorization. Presented at *3th International Conference on Large-Scale Scientific Computation*. (Sozopol, Bulgaria, 2021-06-07 - 2021-06-07). (LA-UR-21-24960)

Alexandrov, B., G. Manzini and E. W. Skau. Nonnegative Canonic Polyadic Decomposition for Tensors with Rank Deficient Factors. Presented at *International Conference on Machine Learning*. (Long Beach, California, United States, 2019-06-10 - 2019-06-15). (LA-UR-19-20517)

Alexandrov, B., I. Djibrilla Boureima, M. Bhattarai, M. E. Eren, E. W. Skau, P. R. Romero and S. J. Eidenbenz. Distributed Out-of-core NMF of Dense and Sparse Data on CPU/GPU Architectures with Automatic Model Selection for Exascale Data. Presented at *36th IEEE International Parallel & Distributed Processing Symposium*. (Lyon, France, 2022-05-30 - 2022-05-30). (LA-UR-21-29812)

Alexandrov, B., K. Kabir, M. Bhattarai and A. Shehu. Single Model Quality Estimation of Protein Structures via Non-negative Tensor Factorization. Presented at *International Conference on Bioinformatics and Biomedicine*. (Houston-virtually, Texas, United States, 2021-12-09 - 2021-12-09). (LA-UR-21-28965)

Alexandrov, B., M. E. Eren, N. Solovyev, C. H. Hamer, R. McDonald and C. Nicholas. COVID-19 Multidimensional Kaggle Literature Organization. Presented at *The ACM Symposium on Document Engineering*. (Limerick, Ireland, 2021-08-24 - 2021-08-24). (LA-UR-21-25094)

Bhattarai, M., G. Chennupati, E. W. Skau, R. Vangara, H. N. Djidjev and B. Alexandrov. Distributed Non-negative Tensor Train Factorization. Presented at *IEEE High-Performance Extreme Computing Conference (HPEC '20)*. (Boston, Massachusetts, United States, 2020-09-22 - 2020-09-24). (LA-UR-20-24426)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics*. (Online, New Mexico, United States, 2020-11-09 - 2020-11-10). (LA-UR-20-26304)

Manzini, G., E. W. Skau, P. M. D. Truong and R. Vangara. Nonnegative tensor-train low-rank approximations of the Smoluchowski equation. Presented at *13th International Conference on "Large-Scale Scientific Computations"*. (Sozopol, Bulgaria, 2021-06-07 - 2021-06-11). (LA-UR-21-23325)

Nasrin, A., R. Vangara, G. Chennupati, B. Alexandrov, H. N. Djidjev and S. Amarda. Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures. Presented at *IEEE International Conference on Bioinformatics and Biomedicine*. (San Diego, California, United States, 2019-11-18 - 2019-11-21). (LA-UR-19-30412)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Optimizing the spin reversal transform on the D-Wave 2000Q. Presented at *ICRC 2019*. (San Mateo, California, United States, 2019-11-06 - 2019-11-08). (LA-UR-19-25307)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Peering into the Anneal Process of a Quantum Annealer. Presented at *PDCAT 2019*. (Gold Coast, Australia, 2019-12-05 - 2019-12-07). (LA-UR-19-27870)

Pulido, J. J., J. M. Patchett, M. Bhattarai, B. Alexandrov and J. P. Ahrens. Selection of Optimal Salient Time Steps by Non-negative Tucker Tensor Decomposition. Presented at *EuroVis 2021 - Conference on Visualization*. (Zurich, Switzerland, 2021-06-14 - 2021-06-18). (LA-UR-21-22070)

Sanchez, G., E. W. Skau and B. Alexandrov. QUATERNION NON-NEGATIVE MATRIX FACTORIZATION WITH MODEL SELECTION FOR SPECTROPOLARIMETRIC IMAGING. Presented at *2021 IEEE International Conference on Acoustics, Speech and Signal Processing*. (Toronto, Canada, 2021-06-06 - 2021-06-11). (LA-UR-20-28403)

Vangara, R., E. W. Skau, G. Chennupati, H. N. Djidjev, M. Bhattarai, T. E. I. Tierney, J. P. Smith, V. Stanev and B. Alexandrov. Finding the Number of Topics with Semantic Nonnegative Matrix Factorization. Presented at *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML PKDD)*

2020. (Ghent, Belgium, 2020-09-14 - 2020-09-18). (LA-UR-20-22845)

Vangara, R., E. W. Skau, G. Chennupati, H. N. Djidjev, T. E. I. Tierney, J. P. Smith, M. Bhattarai, V. Stanev and B. Alexandrov. Semantic Nonnegative Matrix Factorization with Automatic Model Determination for Topic Modeling. Presented at *19th IEEE International Conference On Machine Learning And Applications*. (MIAMI, Florida, United States, 2020-12-14 - 2020-12-17). (LA-UR-20-28028)

Reports

Alexandrov, B., G. Manzini, E. W. Skau and P. M. D. Truong. Composite numerical integration on the multidimensional hypercube using low-rank tensor-train cross representation. Unpublished report. (LA-UR-21-24664)

Alexandrov, B., M. E. EREN, M. Bhattarai, R. J. JOYCE, E. RAFF and C. NICHOLAS. Semi-supervised Classification of Malware Families via Hierarchical Non-negative Matrix Factorization with Automatic Model Determination. Unpublished report. (LA-UR-21-29919)

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. distNMFk: Distributed Non-negative Matrix Factorization to Extract Optimal Number of Features. Unpublished report. (LA-UR-19-25810)

DeSantis, D. F., L. Van Roekel, B. Alexandrov and R. Vangara. Hidden Climate Signatures and Mechanisms in Energy Exascale Earth System Model Data. Unpublished report. (LA-UR-21-21294)

Presentation Slides

Ahmmed, B. Numerical Modeling, Uncertainty Analyses, and Machine Learning for Decision Support in the Geosciences. . (LA-UR-20-23178)

Ahmmed, B. Supervised and Unsupervised Machine Learning to Understanding Reactive-transport Data. . (LA-UR-20-23812)

Ahmmed, B., N. Lautze, V. V. Vesselinov, D. Dores and M. K. Mudunuru. Unsupervised Machine Learning to Extract Dominant Geothermal Attributes\xc2\xa0in Hawaii Island Play Fairway Data. Presented at *Geothermal Resources Council*, Reno, Nevada, United States, 2020-10-18 - 2020-10-23. (LA-UR-20-26170)

Ahmmed, B., V. V. Vesselinov and M. K. Mudunuru. Non-negative Matrix Factorization to Discover Dominant Attributes in Utah FORGE Data. Presented at *Geothermal Resources Conference*, Reno, Nevada, United States, 2020-10-18 - 2020-10-23. (LA-UR-20-26171)

Ahmmed, B., V. V. Vesselinov and M. K. Mudunuru. Machine Learning to Characterize Regional Geothermal Reservoirs in the Western USA. Presented at *GSA*, Online, Colorado, United States, 2020-10-26 - 2020-10-30. (LA-UR-20-27654)

Alexandrov, B. Unsupervised Phase Mapping of X-ray Diffraction Data by Nonnegative Matrix Factorization. Presented at

Invited talk in UC Irvine University on AI and Materials, Irvine, California, United States, 2019-11-21 - 2019-11-21. (LA-UR-19-31561)

Alexandrov, B. Nonnegative Tensor Nets and Extraction of Latent Variables Targeting Discovery. . (LA-UR-20-25418)

Alexandrov, B. Scientific Leadership Identification and Characterization. Presented at *ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING FOR IAEA SAFEGUARDS*, Virtual, New York, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22273)

Alexandrov, B., E. M. Kober and R. Vangara. Tensor Factorization for Chemical Reactions Analysis. Presented at *Machine Learning in Chemical and Materials Sciences*, Los Alamos National, New Mexico, United States, 2021-05-12 - 2021-05-12. (LA-UR-21-24533)

Alexandrov, B., G. Manzini, E. W. Skau, P. M. D. Truong and R. Vuchkov. Tensor Train Network and its Applications to Numerical Integration and Partial Differential Equations. Presented at *Optimization Seminar, University of California, Merced*, Merced, California, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-29268)

Alexandrov, B. and G. Manzini. Tensor Networks Application to Numerical Integration. . (LA-UR-21-32428)

Alexandrov, B. and T. Mina. Test with Gaussian signals. . (LA-UR-20-24155)

Bhattarai, M., G. Chennupati, E. W. Skau, R. Vangara, H. N. Djidjev and B. Alexandrov. Distributed Non-Negative Tensor Train Decomposition. Presented at *IEEE High Performance Extreme Computing Conference (HPEC '20)*, Boston, Massachusetts, United States, 2020-09-21 - 2020-09-25. (LA-UR-20-27354)

Chennupati, G. Massively Parallel Big-Data Nonnegative Factorization. Presented at *Internal DR appraisal review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21162)

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. Distributed Non-negative Matrix Factorization with Model Determination. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Los Alamos, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29294)

Eren, M. E., J. S. Moore and B. Alexandrov. Anomalous Event Detection using Non-Negative Poisson Tensor Factorization. . (LA-UR-20-25933)

Eren, M. E., J. S. Moore and B. Alexandrov. Anomalous Event Detection using Non-Negative Poisson Tensor Factorization. . (LA-UR-20-26093)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics (ISI)*, Online, New Mexico, United States, 2020-11-09 - 2020-11-10. (LA-UR-20-28568)

Eren, M. E., J. S. Moore and B. Alexandrov. Multi-Dimensional Anomalous Entity Detection via Poisson Tensor Factorization. Presented at *IEEE Intelligence and Security Informatics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-10. (LA-UR-20-28561)

Kober, E. M., M. F. Francis, R. Vangara and B. Alexandrov. Tensor Factorization Applied to the Reaction Analysis of Energetic Materials. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29243)

Manzini, G. A non-negative tensor-train based method for the Smoluchowski coagulation equation.. Presented at *13th International Conference on Large-Scale Scientific Computations*, Sozopol, Bulgaria, 2021-06-07 - 2021-06-11. (LA-UR-21-25537)

Marcillo, O. E. and J. K. MacCarthy. Mapping Tonal Noise in the Continental US. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29507)

Nebgen, B. T., J. K. MacCarthy and B. Alexandrov. Non-Negative Tensor Factorization for Interpretable Unsupervised Signal Discovery in Continuous Seismic Data. Presented at *Seismological Society of America National Meeting*, Seattle, Washington, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23443)

Nebgen, B. T., R. Vangara, S. Kuksova, M. A. Hombrados Herrera and B. Alexandrov. Machine Learning for Automated Feature Recognition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29238)

O'Malley, D. Tensor factorization with quantum annealing. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29405)

Skau, E. W. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29328)

Skau, E. W., M. Bhattarai, N. S. Kharat, G. Chennupati, R. Vangara, S. Rajopadhye, H. N. Djidjev and B. Alexandrov. Distributed Non-Negative RESCAL for Heterogeneous Architectures with Model Determination. Presented at *SIAM Conference on Applied Linear Algebra (LA21)*, Los Alamos, New Mexico, United States, 2021-05-17 - 2021-05-21. (LA-UR-21-24880)

Vangara, R., B. T. Nadiga and B. Alexandrov. Tensor Methods for analyzing Sea Ice Thickness in Arctic.. Presented at *AI4ESP*, Los Alamos, New Mexico, United States, 2021-01-08 - 2021-01-08. (LA-UR-21-20130)

Vesselinov, V. V. Physics-Informed Machine Learning Methods for Data Analytics and Model Diagnostics. Presented at *M3 DRIVE Science Center:*, Los Alamos, New Mexico, United States, 2019-05-14 - 2019-05-14. (LA-UR-19-24562)

Vesselinov, V. V., B. Ahmmed and M. K. Mudunuru. Unsupervised Machine Learning to discover attributes that characterize low, moderate, and high-temperature geothermal resources. Presented at *Geothermal Resources Conference*, Reno, Nevada, United States, 2020-10-18 - 2020-10-23. (LA-UR-20-26184)

Posters

Bhattarai, M., R. Vangara, G. Chennupati, J. M. Patchett, J. P. Ahrens and B. Alexandrov. pyDnMFk: A Python implementation of Distributed Non-Negative Matrix Factorization with determination of Rank. Presented at *LDRD Project Review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21243)

Carrillo Cabada, H. A., E. W. Skau, G. Chennupati, H. N. Djidjev and B. Alexandrov. Out-of-Core Singular Value Decomposition for the Tensor Train Decomposition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29330)

Carrillo, H., E. W. Skau, G. Chennupati, H. N. Djidjev and B. Alexandrov. Out-of-Core Singular Value Decomposition for the Tensor Train Decomposition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29862)

Francis, M. F., E. M. Kober, B. Alexandrov, R. Vangara and B. T. Nebgen. Machine Learning of Transient Chemical Kinetics: NMF, NN, and SVR of HMX. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29274)

Hombrados Herrera, M. A., R. Vangara, E. W. Skau and B. Alexandrov. Methods for determination of dimensionality of latent features: Principal Angles and PCAk. Presented at *AI and Tensor Factorizations for Physical, Chemical and Biological Systems.*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-19. (LA-UR-19-29467)

Kuksova, S., B. Alexandrov and K. O. Rasmussen. Nonegative Tensor Train Analysis for Feature Extraction. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29464)

M. Mallory, E. J., B. T. Nebgen, O. E. Marcillo, J. K. MacCarthy, K. O. Rasmussen and B. Alexandrov. Tensor Decomposition for Mars Seismology. Presented at *Elizabeth Mallory*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29281)

M. Mallory, E. J., T. B. Peery and M. F. Francis. Statistical Representations and Unbiased Metrics for Stable Isotope Fractionation. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32132)

Nasrin, A., R. Vangara, G. Chennupati, B. Alexandrov, H. N. Djidjev and S. Amarda. Non-Negative Matrix Factorization for Decoy Selection from Ensembles. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Los Alamos, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29332)

Rasmussen, K. O., E. J. M. Mallory, B. T. Nebgen, O. E. Marcillo, J. K. MacCarthy and B. Alexandrov. Tensor Decomposition for Mars Seismology. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, SANTA FE, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29777)

Rasmussen, K. O., G. Bel, R. Vangara, D. Petsev and B. Alexandrov. Unsupervised Learning for Anomalous Diffusion Source Identification. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29256)

Rasmussen, K. O., S. Kuksova and B. Alexandrov. Nonnegative Tensor Train Analysis for Feature Extraction. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29776)

Rijal, B., B. T. Nebgen, C. A. Neale and B. Alexandrov. Tensor Factorization for Protein Conformation Identification. Presented at *AI and Tensor Factorization for Physical, Chemical and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29311)

Skau, E. W. Symmetric Tucker Rank Determination. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29329)

Truong, D., E. W. Skau and B. Alexandrov. Symmetric Tucker Rank Determination. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29863)

Vangara, R., E. M. Kober and B. Alexandrov. Tensor Methods for Reaction Analysis of Energetic Materials and High Explosives. Presented at *DR Midterm Review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21230)

Vangara, R., G. Chennupati and B. Alexandrov. Symmetric Non-Negative Matrix Factorization with PAC for Estimating Number of Clusters. Presented at *Conference on Data Analysis (CODA 2020)*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21809)

Machine Learning for Turbulence

Daniel Livescu
20190059DR

Project Description

Machine Learning for Turbulence will develop a novel framework which will dramatically improve models used in hydrodynamic codes at Los Alamos National Laboratory and other National Laboratories of the Department of Energy. The models are significant for such mission critical applications as weapons design and simulations, modeling and predictive weather and understanding astrophysical phenomena. Our main hypothesis is that an automatic design of the hydrodynamic closures is achievable through new approach, coined Physics Informed Machine Learning, suggesting and developing smart embedding of the underlying physics into Machine Learning techniques. We will test the hypothesis by developing a theoretical and algorithmic methods guided by insight from the hydrodynamic applications of interest. We will examine the power of the new tools in bridging existing approaches. Thus, application agnostic machine learning will be augmented with the physical constraints reflecting basic hydrodynamic symmetries. Complementary, current Laboratory closure models of turbulence will be enhanced by embedding into them Neural Networks thus allowing automatic evaluation, larger time steps and faster in line computations.

Technical Outcomes

The project has made a broad range of important contributions to the structure of neural networks and differential programming, as well as novel applications to turbulence modeling in Lagrangian framework, memory effects, dynamical regime identification, and graphical models. The project has also made contributions to climate and astrophysics applications. Several methods developed by the project have been adopted in Laboratory programs (such as Advanced Simulation and Computing; Office of Experimental Sciences, climate) and new funding was obtained to further develop other project methods.

Publications

Journal Articles

Andrassy, R., J. Higl, H. Mao, M. Moc\xc3\xa1k, D. G. Vlaykov, I. Baraffe, S. W. Campbell, T. Constantino, P. V. F. Edelmann, T. Goffrey, T. Guillet, F. Herwig, R. Hirschi, L. Horst, G. Leidi, J. Pratt, F. K. R\xc3\xb6pke and P. Woodward. Dynamics in a stellar convective layer and at its boundary: Comparison of five 3D hydrodynamics codes. Submitted to *Astronomy and Astrophysics*. (LA-UR-21-25840)

*Andrews, S., C. Fryer, W. Even, S. Jones and M. Pignatari. The Nucleosynthetic Yields of Core-collapse Supernovae: Prospects for the Next Generation of Gamma-Ray Astronomy. 2020. *The Astrophysical Journal*. **890** (1): 35. (LA-UR-19-30411 DOI: 10.3847/1538-4357/ab64f8)

Chertkov, M., M. Escobar Santoro and D. Bienstock. Learning from power system data stream: phasor - detective approach. Submitted to *Arvix*. (LA-UR-18-30924)

Chertkov, M., V. Y. Chernyak and Y. Maximov. Gauges, Loops, and Polynomials for Partition Functions of Graphical Models. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-20-30432)

*Chertkov, M. and Y. Maximov. Gauges, loops, and polynomials for partition functions of graphical models. 2020. *Journal of Statistical Mechanics: Theory and Experiment*. **2020** (12): 124006. (LA-UR-18-30593 DOI: 10.1088/1742-5468/abcaf0)

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Automated identification of dominant physical processes through machine learning. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-22-20119)

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Automated identification of dominant physical processes. Submitted to *Nature Machine Intelligence*. (LA-UR-22-20935)

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

*Likhosherstov, V., Y. Maximov and M. Chertkov. Tractable minor-free generalization of planar zero-field Ising models. 2020. *Journal of Statistical Mechanics: Theory*

and Experiment. **2020** (12): 124007. (LA-UR-19-30102 DOI: 10.1088/1742-5468/abcaf1)

Lin, Y. T., Y. Tian, M. Anghel and D. Livescu. Data-driven learning for the Mori--Zwanzig formalism: a generalization of the Koopman learning framework. Submitted to *SIAM Journal on Applied Dynamical Systems*. (LA-UR-21-20187)

*Maulik, R., A. T. Mohan, B. Lusch, S. Madireddy, P. Balaprakash and D. Livescu. Time-series learning of latent-space dynamics for reduced-order model closure. 2020. *Physica D: Nonlinear Phenomena*. **405**: 132368. (LA-UR-19-28714 DOI: 10.1016/j.physd.2020.132368)

Mohan, A. T., D. Daniel, M. Chertkov and D. Livescu. COMPRESSED CONVOLUTIONAL LSTM: AN EFFICIENT DEEP LEARNING FRAMEWORK TO MODEL HIGH FIDELITY 3D TURBULENCE. Submitted to *Arxiv*. (LA-UR-19-21568)

Mohan, A. T., K. Nagarajan and D. Livescu. Learning Galerkin models of Turbulence with Differentiable Programming. Submitted to *Journal of Fluid Mechanics*. (LA-UR-21-26236)

Mohan, A. T., N. E. Lubbers, D. Livescu and M. Chertkov. Embedding Hard Physical Constraints in Neural Network Coarse-Graining of 3D Turbulence. Submitted to *Physical Review Fluids*. (LA-UR-20-20560)

Nadiga, B. T. Machine Learning as a Tool for Climate Predictability Studies. Submitted to *Journal of Advances in Modeling Earth Systems*. (LA-UR-20-26537)

Nouri, A. G., H. Babaee, P. Givi, H. Chelliah and D. Livescu. Skeletal model reduction with forced optimally time dependent modes. 2021. *Combustion and Flame*. 111684. (LA-UR-21-22082 DOI: 10.1016/j.combustflame.2021.111684)

Portwood, G. D., B. T. Nadiga, J. A. Saenz and D. Livescu. Diagnostics and interprettability of out-performing artificial neural network residual flux models. Submitted to *Journal of Fluid Mechanics Rapids*. (LA-UR-20-20405)

Portwood, G. D., S. de Bruyn Kops, E. Rietman and D. Saunders. Unsupervised Machine Learning to Teach Fluid Dynamicists to Think in 15 Dimensions. Submitted to *Journal of Turbulence*. (LA-UR-19-27313)

Portwood, G. D., S. de Bruyn Kops and C. Caulfield. Implications of inertial subrange scaling on stably stratified mixing. Submitted to *Journal of Fluid Mechanics*. (LA-UR-20-28841)

Portwood, G. D. and S. de Bruyn Kops. Idealized Turbulent Wake With Steady, Non-Uniform Ambient Density Stratification. Submitted to *Journal of Fluid Mechanics*. (LA-UR-20-28846)

*Pulido, J., R. D. da Silva, D. Livescu and B. Hamann. Multiresolution classification of turbulence features in image data through machine learning. 2021. *Computers & Fluids*. **214**: 104770. (LA-UR-19-31868 DOI: 10.1016/j.compfluid.2020.104770)

Shankar, V., G. D. Portwood, A. T. Mohan, P. P. Mitra, D. Krishnamurthy, C. Rackauckas, L. A. Wilson, D. P. Schmidt and V. Viswanathan. Physics-constrained neural dynamics

model for turbulent fluid flow. Submitted to *Physical Review Fluids*. (LA-UR-21-27558)

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

Tian, Y., D. Livescu and M. Chertkov. Physics-informed Machine Learning of the Lagrangian Dynamics of Velocity Gradient Tensor. Submitted to *Physical Review Fluids*. (LA-UR-20-29349)

Tian, Y., Y. T. Lin, M. Anghel and D. Livescu. Data Driven Learning of Mori-Zwanzig Operators for Isotropic Turbulence. Submitted to *Physics of Fluids*. (LA-UR-21-28283)

Conference Papers

Bas, E. E., D. Aslangil and M. A. Moustafa. PREDICTING NONLINEAR SEISMIC RESPONSE OF STRUCTURAL BRACES USING MACHINE LEARNING. Presented at *ASME, International Mechanical Engineering Congress and Exposition (IMECE), 2020*. (Portland, Oregon, United States, 2020-11-15 - 2020-11-19). (LA-UR-20-23613)

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

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

Jayakumar, A., A. Lokhov, S. Misra and M. D. Vuffray. Learning of Discrete Graphical Models with Neural Networks. Presented at *NeurIPS*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-24927)

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

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

Mohan, A. T., D. Livescu and M. Chertkov. Wavelet-Powered Neural Networks for Turbulence. Presented at *33rd Conference on Neural Information Processing Systems (NeurIPS)*. (Vancouver, Canada, 2019-12-14 - 2019-12-14). (LA-UR-19-31274)

Shankar, V., G. D. Portwood, A. T. Mohan, P. P. Mitra, C. Rackauckas, L. Wilson, D. Schmidt and V. Vishwanathan. Non-Linear Dynamics Learning using Convolutional Neural

ODEs. Presented at *NeuRIPS Conference*. (Vancouver, Canada, 2020-12-06 - 2020-12-12). (LA-UR-20-27785)

Su, X., R. Walters, D. Aslangil and R. Yu. FORECASTING VARIABLE-DENSITY 3D TURBULENT FLOW. Presented at *Simulation with Deep Learning (SimDL) International Conference on Learning Representations (ICLR) Workshop*. (Vienna (virtual), Austria, 2021-05-04 - 2021-05-08). (LA-UR-21-22738)

Tano, M. and G. D. Portwood. Accelerating training in artificial neural networks with dynamic mode decomposition. Presented at *NeurIPS 2020*. (Vancouver (or Virtual), Canada, 2020-12-06 - 2020-12-12). (LA-UR-20-24004)

Theiler, J. P. and C. X. Ren. Distilled Gaussianization. Presented at *SPIE Optics+Photonic Symposium: Applications of Machine Learning Conference*. (Santa Fe, New Mexico, United States, 2021-08-01 - 2021-08-05). (LA-UR-21-27231)

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

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *NeurIPS 2020*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-25018)

Reports

Belyy, A., A. Sholokhov, M. R. Amini and Y. Maximov. MEMOIR: Multi-class Extreme Classification with Inexact Margin. Unpublished report. (LA-UR-19-21219)

Chertkov, M., Y. Maximov and V. LIkhosherstov. Inference and Sampling of K(3,3)-free Ising Models. Unpublished report. (LA-UR-18-31783)

Crum, J. R. LANL MELT Project. Unpublished report. (LA-UR-19-27901)

Kaiser, B. E., J. A. Saenz, M. J. Sonnewald and D. Livescu. Solving the dynamical regime problem: A new era of discovery guided by machine learning. Unpublished report. (LA-UR-21-25813)

Krechetov, M., Y. Maximov, J. Marecek and M. Takac. Entropy-Penalized Semidefinite Programming. Unpublished report. (LA-UR-18-24430)

Likhosherstov, V., Y. Maximov and M. Chertkov. Inference and Sampling of K33-free Ising Models. Unpublished report. (LA-UR-19-26932)

Likhosherstov, V., Y. Maximov and M. Chertkov. A New Family of Tractable Ising Models. Unpublished report. (LA-UR-19-24712)

Mohan, A. T. IC Project Report: Machine Learning for Turbulence. Unpublished report. (LA-UR-21-24516)

Woodward, M. J., Y. Tian, C. M. Hyett, C. L. Fryer, D. Livescu, M. Stepanov and M. Chertkov. Physics Informed Machine Learning of SPH: Machine Learning Lagrangian Turbulence. Unpublished report. (LA-UR-21-30101)

Presentation Slides

Aslangil, D. Denis Aslangil web-page contents (denisaslangil.com). . (LA-UR-20-20826)

Chakrabarti, S., A. T. Mohan, D. Livescu and D. Gaitonde. Galerkin Reduced Order Models for Compressible Flows with Differentiable Programming. Presented at *APS DFD*, Phoenix, Arizona, United States, 2021-11-21 - 2021-11-23. (LA-UR-21-31515)

Kaiser, B. E., J. A. Saenz and D. Livescu. Leading-Order Analysis by Artificial Intelligence. . (LA-UR-20-27102)

Kaiser, B. E., J. A. Saenz and D. Livescu. Empirical Leading-Order Analysis by Artificial Intelligence. . (LA-UR-20-29032)

Livescu, D. LDRD DR – MELT: Machine Learning for Turbulence. . (LA-UR-20-20578)

Livescu, D. Machine Learning for Turbulence. . (LA-UR-22-20657)

Maulik, R., A. T. Mohan, S. Madireddy, B. Lusch, P. Balaprakash and D. Livescu. MACHINE LEARNING OF SEQUENTIAL DATA FOR REDUCED ORDER MODELS. Presented at *APS DFD 2019*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31882)

Mitra, P. P. and G. D. Portwood. Improving climate sub-closures with ML. Presented at *NVIDIA GTC 2020: Deep Learning & AI Conference*, San Jose, California, United States, 2020-03-22 - 2020-03-26. (LA-UR-19-29812)

Mohan, A. T. Deep Learning for Efficient Modeling of High Dimensional Spatiotemporal Physics. Presented at *Nvidia GTC Conference 2020*, San Jose, California, United States, 2020-03-23 - 2020-03-26. (LA-UR-20-21748)

Mohan, A. T. Machine Learning for Turbulence. . (LA-UR-21-24513)

Mohan, A. T. HARPI: Hybrid AI for Next Generation Resilient Piping. Presented at *LANL DisrupTech*, Los Alamos, New Mexico, United States, 2021-08-18 - 2021-08-18. (LA-UR-21-28263)

Mohan, A. T., D. Livescu and M. Chertkov. Physics-Constrained Convolutional-LSTM Networks for Generative Modeling of Turbulence. Presented at *APS DFD 2019*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31836)

Mohan, A. T., K. Nagarajan and D. Livescu. Learning Physics-based Galerkin models of turbulence with Neural Differential Equations. Presented at *American Physical Society, Division of Fluid Dynamics annual meeting*, Chicago, Illinois, United States, 2020-11-22 - 2020-11-22. (LA-UR-20-29643)

Nadiga, B. T. Learning Spatiotemporal Variability of Climate. Presented at *APS DFD 2019*, Seattle, Washington, United States, 2019-11-23 - 2019-11-23. (LA-UR-19-31764)

Nadiga, B. T., C. Jiang and A. B. Farimani. PREDICTING INTERANNUAL VARIABILITY OF CLIMATE USING DEEP LEARNING. Presented at *APS DFD, Climate Informatics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-23. (LA-UR-19-27540)

Nadiga, B. T. and D. Livescu. Leveraging Bayesian Analysis to Improve Accuracy of the BHR3 Turbulence Model. Presented at *NEDPC*, Los Alamos, New Mexico, United States, 2019-10-14 - 2019-10-14. (LA-CP-19-20678)

Portwood, G. D. Interpretable artificial neural networks outperform canonical LES closures. Presented at *Universality: Turbulence Across Vast Scales*, New York, New York, United States, 2019-12-02 - 2019-12-06. (LA-UR-19-31795)

Portwood, G. D. Multi-paradigm data-driven turbulence and mixing modeling with artificial neural networks: Methodologies,\xc2\xa0diagnostics, and \xc2\xa0interpretability. Presented at *Machine Learning for Turbulence LDRD Program Review*, Santa Fe, New Mexico, United States, 2020-01-17 - 2020-01-17. (LA-UR-20-20438)

Portwood, G. D. Multi-paradigm data-driven turbulence modeling with artificial neural networks. Presented at *Department of Defense High Performance Computing Modernization Program Talk*, Vicksburg, Mississippi, United States, 2020-02-12 - 2020-02-12. (LA-UR-20-21319)

Portwood, G. D. Harmonious integration of Deep ML with fluid simulation and modeling. Presented at *ICLR 2020*, Virtual, New Mexico, United States, 2020-04-26 - 2020-04-26. (LA-UR-20-22993)

Portwood, G. D. Machine Learning for Computational Fluid Dynamics. Presented at *NeurIPS 2020*, Virtual, New Mexico, United States, 2020-12-06 - 2020-12-12. (LA-UR-20-24583)

Portwood, G. D., J. A. Saenz, B. T. Nadiga, D. Livescu and M. Chertkov. Physics-informed deep neural networks applied to scalar subgrid flux modeling in a mixed DNS/LES framework. Presented at *APS Division of Fluid Dynamics 2019*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31769)

Portwood, G. D., J. A. Saenz and S. M. de Bruyn Kops. Identification and parametrization of spontaneous shear instabilities in stratified turbulence via convolutional neural networks. Presented at *17th European Turbulence Conference*, Torino, Italy, 2019-09-03 - 2019-09-06. (LA-UR-19-29104)

Portwood, G. D., P. P. Mitra, M. Dias Ribeiro and T. Nguyen. Improving geophysical turbulence models with NeuralODE. Presented at *GPU Technology Conference 2020*, Virtual, California, United States, 2020-03-23 - 2020-03-23. (LA-UR-20-22381)

Praturi, D. S. and A. T. Mohan. Analyses of Differential-programming Paradigm for Learning Physics-constrained Surrogate Models. Presented at *APS DFD 2021*, Phoenix, Arizona, United States, 2021-11-21 - 2021-11-23. (LA-UR-21-31516)

Ribeiro, M. D., G. D. Portwood, P. P. Mitra, T. M. Nguyen, B. T. Nadiga, M. Chertkov, A. Anandkumar and D. Schmidt. A data-driven approach to modeling turbulent decay at non-asymptotic Reynolds numbers. Presented at *APS Division of Fluid Dynamics 2019*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31772)

Tian, Y., D. Livescu and M. Chertkov. Physics Informed Learning of Lagrangian Turbulence: Velocity Gradient Tensor. Presented at *APS Division of Fluid Dynamics Annual Meeting*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31590)

Tian, Y., M. J. Woodward, C. M. Hyett, M. Stepanov, C. L. Fryer, D. Livescu and M. Chertkov. Machine learning Lagrangian turbulence models based on smoothed particle hydrodynamics. Presented at *APS Division of Fluid Dynamics Meeting*, Phoenix, Arizona, United States, 2021-11-21 - 2021-11-23. (LA-UR-21-31506)

Tian, Y., Y. T. Lin, M. Anghel and D. Livescu. Data-driven learning of Mori-Zwanzig Operator for isotropic turbulence. Presented at *APS Division of Fluid Dynamics Meeting*, Phoenix, Arizona, United States, 2021-11-21 - 2021-11-23. (LA-UR-21-31512)

Z. Towery, C. A., J. A. Saenz and D. Livescu. A comparison of hybrid RANS/LES models across the complete transition from URANS to DNS. Presented at *74th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Phoenix, Arizona, United States, 2021-11-21 - 2021-11-23. (LA-UR-21-31352)

Z. Towery, C. A., J. A. Saenz and D. Livescu. A comparison of hybrid RANS/LES models across the complete transition from URANS to DNS. Presented at *74th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Phoenix, Arizona, United States, 2021-11-21 - 2021-11-23. (LA-UR-21-31457)

Tretiak, D. S., A. T. Mohan and D. Livescu. Embedding Physics In Generative Adversarial Networks for 3D Turbulence. Presented at *APS Division of Fluid Dynamics Annual Meeting*, Chicago (virtual), Illinois, United States, 2020-11-22 - 2020-11-24. (LA-UR-20-29581)

Vuffray, M. D. Efficient Learning of Discrete Graphical Models. Presented at *Graphical models, Exchangeable models and Graphons*, Cambridge, Massachusetts, United States, 2019-08-18 - 2019-08-21. (LA-UR-19-28437)

Posters

Anghel, M. and Y. T. Lin. A Mori-Zwanzig Approach to Data Fusion and Optimal Prediction. Presented at *Data and Information Fusion Conference*, Santa Fe, New Mexico, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28345)

Aslangil, D., D. Livescu and A. Banerjee. DYNAMICS OF TURBULENCE WITH LARGE DENSITY VARIATIONS. Presented

at *International Mechanical Engineering Congress & Exposition*, Salt Lake City, Utah, United States, 2019-11-11 - 2019-11-15. (LA-UR-19-31454)

King, R., O. A. Hennigh, A. T. Mohan and M. Chertkov. From Deep to Physics-Informed Learning of Turbulence: Diagnostics. Presented at *Neural Information Processing Systems*, Montreal, Canada, 2018-12-03 - 2018-12-08. (LA-UR-18-31549)

Nadiga, B. T., J. R. Urrego Blanco and M. A. Taylor. Nonlinear Evolution of a BaroclinicWave and Imbalanced Dissipation. Presented at *Atmosphere and Oceanic Fluid Dynamics*, Portland, Maine, United States, 2019-06-27 - 2019-06-27. (LA-UR-19-26320)

Portwood, G. D., J. A. Saenz, B. T. Nadiga and D. Livescu. Out-performing algebraic residual flux models in Large Eddy Simulations using artificial neural networks. Presented at *NSF Workshop on Exuberance of Machine Learning in Transport Phenomena*, Dallas, Texas, United States, 2020-02-10 - 2020-02-11. (LA-UR-20-21257)

Portwood, G. D., J. A. Saenz and D. Livescu. Autonomous RANS/LES hybrid models enabled by machine-learned subclosures. . (LA-UR-19-28662)

Portwood, G. D., P. P. Mitra, M. Dias Ribeiro, T. Nguyen, B. T. Nadiga, J. A. Saenz, A. Amandkumar and D. Schmidt. Turbulence Forecasting via Neural ODEs. Presented at *GPU Technology Conference (NVidia)*, Santa Clara, California, United States, 2020-03-22 - 2020-03-26. (LA-UR-19-30802)

Portwood, G. D., P. P. Mitra, M. Dias Ribeiro, T. Nguyen, B. T. Nadiga, J. A. Saenz, M. Cherkov, A. Garg, A. Anandkumar, A. Dengel, R. Baraniuk and D. Schmidt. Turbulence Forecasting via Neural ODEs. Presented at *NeurIPS 2019 Workshop on Machine Learning and the Physical Sciences*, Vancouver, Canada, 2019-12-13 - 2019-12-14. (LA-UR-19-31796)

Tretiak, D. S., A. T. Mohan, D. Livescu and M. Chertkov. Applying GANs to the Problem of Turbulence. . (LA-UR-20-23676)

Taming Defects in Quantum Computers

Scott Pakin
20190065DR

Project Description

Since the enactment of the Comprehensive Nuclear Test Ban Treaty, stockpile stewardship has relied heavily on computer simulations of weapons effects. Until recently, continuous improvements in supercomputing technology have made it possible to increase the physics fidelity of these simulations without unduly slowing them down. Alas, with all of the low-hanging fruit long since picked, performance improvements are becoming increasing elusive with each new generation of supercomputers. The situation existentially threatens the National Nuclear Security Administration's ability to ensure the safety, security, and effectiveness of America's nuclear stockpile. Quantum computing is a new technology that offers the potential of drastically improved computational speed—well beyond what any supercomputer in the foreseeable future is capable of. Unfortunately, early quantum computers are extremely unreliable and extremely difficult to program. Our project will address both those issues. We will develop a framework that enables NNSA computational scientists to describe a mapping of inputs to outputs and automatically converts that mapping into a quantum algorithm, and one that is customized to work around a particular quantum computer's individual shortcomings. This will enable stockpile stewardship simulations to continue their prior trajectory of ever-improving accuracy and ever-improving utility to national security.

Technical Outcomes

From a research and development standpoint, the project was a resounding success. It laid a general framework for noise mitigation, provided new understanding into the limits of machine learnability in a quantum-computing context, made it possible to perform computations today that would otherwise require many generations of quantum computers before becoming practical, and advanced fundamental knowledge of quantum information science. An unexpected achievement was using project-developed software to win the Fall 2020 IBM Quantum Challenge.

Publications

Journal Articles

Arrasmith, A. T., L. Cincio, R. D. Somma and P. J. Coles. Operator Sampling for Shot-frugal Optimization in Variational Algorithms. Submitted to *npj Quantum Information*. (LA-UR-20-22810)

*Arrasmith, A., L. Cincio, A. T. Sornborger, W. H. Zurek and P. J. Coles. Variational consistent histories as a hybrid algorithm for quantum foundations. 2019. *Nature Physics*. **10** (1): 3438. (LA-UR-18-31704 DOI: 10.1038/s41467-019-11417-0)

Barbosa, A., E. A. R. Pelofske, G. Hahn and H. N. Djidjev. Using machine learning for quantum annealing accuracy prediction. Submitted to *MDPI Special Issue "Quantum Optimization and Machine Learning"*. (LA-UR-21-25091)

Beckey, J., A. Sone, M. V. S. Cerezo de la Roca and P. J. Coles. Variational Quantum Fisher Information Estimation. Submitted to *Quantum*. (LA-UR-20-28328)

Bravo-Prieto, C., R. LaRose, M. V. S. Cerezo de la Roca, Y. Subasi, L. Cincio and P. J. Coles. Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems. Submitted to *arXiv*. (LA-UR-19-29101)

Caro, M., H. Huang, M. V. S. Cerezo de la Roca, K. Sharma, A. T. Sornborger, L. Cincio and P. J. Coles. Generalization in quantum machine learning from few training data. Submitted to *Nature Physics*. (LA-UR-21-31086)

Cerezo, M., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation. 2020. *Quantum*. **4**: 248. (LA-UR-19-25585 DOI: 10.22331/q-2020-03-26-248)

*Cerezo, M., A. Sone, T. Volkoff, L. Cincio and P. J. Coles. Cost function dependent barren plateaus in shallow parametrized quantum circuits. 2021. *Nature Communications*. **12** (1): 1791. (LA-UR-19-32681 DOI: 10.1038/s41467-021-21728-w)

*Charalampidis, E. G., J. F. Dawson, F. Cooper, A. Khare and A. Saxena. Stability and response of trapped solitary wave solutions of coupled nonlinear Schr

\xc3\xb6dinger equations in an external, $\mathcal{PT}$- and supersymmetric potential. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (45): 455702. (LA-UR-20-22820 DOI: 10.1088/1751-8121/abb278)

*Chen, Y., G. Watanabe, Y. Yu, X. Guan and A. del Campo. An interaction-driven many-particle quantum heat engine and its universal behavior. 2019. *npj Quantum Information*. **5** (1): 88. (LA-UR-19-20147 DOI: 10.1038/s41534-019-0204-5)

*Chernyak, V. Y., N. A. Sinitsyn and C. Sun. Dynamic spin localization and \xce\xb3-magnets. 2019. *Physical Review B*. **100** (22): 224304. (LA-UR-19-24184 DOI: 10.1103/PhysRevB.100.224304)

*Chodos, A. and F. Cooper. Neutrino condensation from a new Higgs-like interaction. 2020. *Physical Review D*. **102** (11): 113003. (LA-UR-20-22766 DOI: 10.1103/PhysRevD.102.113003)

*Chowdhury, A. N., R. D. Somma and Y. Subasinodot. Computing partition functions in the one-clean-qubit model. 2021. *Physical Review A*. **103** (3): 032422. (LA-UR-19-30447 DOI: 10.1103/PhysRevA.103.032422)

*Christov, I. C., R. J. Decker, A. Demirkaya, V. A. Gani, P. G. Kevrekidis, A. Khare and A. Saxena. Kink-Kink and Kink-Antikink Interactions with Long-Range Tails. 2019. *Physical Review Letters*. **122** (17): 171601. (LA-UR-18-30946 DOI: 10.1103/PhysRevLett.122.171601)

*Christov, I. C., R. J. Decker, A. Demirkaya, V. A. Gani, P. G. Kevrekidis and A. Saxena. Kink-antikink collisions and multi-bounce resonance windows in higher-order field theories. 2021. *Communications in Nonlinear Science and Numerical Simulation*. **97**: 105748. (LA-UR-20-23167 DOI: 10.1016/j.cnsns.2021.105748)

Cincio, L., K. Rudinger, M. Sarovar and P. J. Coles. Machine Learning of Noise-Resilient Quantum Circuits. 2021. *PRX Quantum*. **2** (1): 010324. (LA-UR-20-24253 DOI: 10.1103/PRXQuantum.2.010324)

Coles, P. J. A separation between classical and quantum neural networks. Submitted to *Nature Computational Science*. (LA-UR-21-24712)

*Coles, P. J., M. Cerezo and L. Cincio. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states. 2019. *Physical Review A*. **100** (2): 022103. (LA-UR-19-22724 DOI: 10.1103/PhysRevA.100.022103)

*Cooper, F., A. Khare, N. R. Quintero, B. Sanchez-Rey, F. G. Mertens and A. Saxena. Parametrically driven nonlinear Dirac equation with arbitrary nonlinearity. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (7): 75203. (LA-UR-19-29780 DOI: 10.1088/1751-8121/ab60e7)

A. A. *. C. P. J. *. C. L. Czarnik, P. *., P. J. Coles, L. Cincio, P. Czarnik and A. Arrasmith. Error mitigation with Clifford quantum-circuit data. 2021. *Quantum*. **5**: 592. (LA-UR-20-23755 DOI: 10.22331/q-2021-11-26-592)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Decomposition Algorithms for Solving NP-hard Problems on a Quantum Annealer. 2021. *Journal of Signal Processing Systems*. **93** (4): 405-420. (LA-UR-19-30809 DOI: 10.1007/s11265-020-01550-1)

Duzgun, A., A. B. Saxena and A. Khare. Explicit Kink Solutions in Several One-Parameter Family of Higher Order Field Theory Models. Submitted to *Journal of Physics A*. (LA-UR-21-22192)

Fontana, E., M. V. S. Cerezo de la Roca, A. T. Arrasmith, I. Runnger and P. J. Coles. Optimizing parameterized quantum circuits via noise-induced breaking of symmetrie. Submitted to *Quantum*. (LA-UR-20-29359)

Geller, M. R., Z. P. Holmes, P. J. Coles and A. T. Sornborger. Experimental Quantum Learning of a Spectral Decomposition. Submitted to *Physical Review A arxiv.org*. (LA-UR-21-22948)

Gibbs, J., K. Gili, Z. P. Holmes, B. Commeau, A. T. Arrasmith, L. Cincio, A. T. Sornborger and P. J. Coles. Long-time simulations with high fidelity on quantum hardware. Submitted to *arXiv, PRX Quantum*. (LA-UR-21-21053)

Holmes, Z. P., K. Sharma, M. V. S. Cerezo de la Roca and P. J. Coles. Connecting ansatz expressibility to cost gradients and barren plateau. Submitted to *Quantum*. (LA-UR-21-20034)

*S. R. *. C. L. *. A. Y. *. B. P. Khairy, S. *. and L. Cincio. Learning to Optimize Variational Quantum Circuits to Solve Combinatorial Problems. 2020. *Proceedings of the AAAI Conference on Artificial Intelligence*. **34** (03): 2367-2375. (LA-UR-19-28945 DOI: 10.1609/aaai.v34i03.5616)

*Khare, A. and A. Saxena. Wide class of logarithmic potentials with power-tower kink tails. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (31): 315201. (LA-UR-19-29212 DOI: 10.1088/1751-8121/ab84ac)

*Khare, A. and A. Saxena. Logarithmic potential with super-super-exponential kink profiles and tails. 2020. *Physica Scripta*. **95** (7): 75205. (LA-UR-19-30366 DOI: 10.1088/1402-4896/ab8eeb)

Khatri, S., R. LaRose, A. Poremba, L. Cincio, A. T. Sornborger and P. J. Coles. Quantum-assisted quantum compiling. 2019. *Quantum*. **3**: 140. (LA-UR-18-25861 DOI: 10.22331/q-2019-05-13-140)

*Kuebler, J. M., A. Arrasmith, L. Cincio and P. J. Coles. An Adaptive Optimizer for Measurement-Frugal Variational Algorithms. 2020. *Quantum*. **4**: 263. (LA-UR-19-29383 DOI: 10.22331/q-2020-05-11-263)

*LaRose, R., A. Tikku, E. O'Neel-Judy, L. Cincio and P. J. Coles. Variational quantum state diagonalization. 2019. *npj Quantum Information*. **5** (1): 57. (LA-UR-18-29266 DOI: 10.1038/s41534-019-0167-6)

Larocca, M., P. J. Czarnik, K. Sharma, G. Muraleedharan, P. J. Coles and M. V. S. Cerezo de la Roca. Diagnosing barren plateaus with tools from quantum optimal

control. Submitted to *Physical Review X Quantum*. (LA-UR-21-24973)

Lu, Q., S. Xie and A. B. Saxena. Theoretical Study on Spin Transport Mechanism in Organic Polymers. Submitted to *Organic Electronics*. (LA-UR-18-30571)

*Nesterov, A. I., G. P. Berman, M. Merkli and A. Saxena. Modeling of noise-assisted quantum transfer between donor and acceptor with finite bandwidths. 2019. *Journal of Physics A: Mathematical and Theoretical*. **52** (43): 435601. (LA-UR-18-31605 DOI: 10.1088/1751-8121/ab4502)

Pakin, S. D. and S. P. Reinhardt. Programming a D-Wave Annealing-Based Quantum Computer: Tools and Techniques. Submitted to *Quantum Information & Computation*. (LA-UR-19-20660)

H. G. *. D. H. Pelofske, E. *., E. Pelofske and H. Djidjev. Inferring the Dynamics of the State Evolution During Quantum Annealing. 2022. *IEEE Transactions on Parallel and Distributed Systems*. **33** (2): 310-321. (LA-UR-20-30193 DOI: 10.1109/TPDS.2020.3044846)

R. Pelofske, E. A., G. Hahn, D. O'Malley, H. N. Djidjev and B. Alexandrov. Boolean Hierarchical Tucker Networks on Quantum Annealers. Submitted to *Large-Scale Scientific Computations*. (LA-UR-21-22363)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Parallel Quantum Annealing. Submitted to *Scientific Reports*. (LA-UR-21-31212)

Pesah, A., M. V. S. Cerezo de la Roca, S. Wang, T. J. Volkoff, A. T. Sornborger and P. J. Coles. Absence of Barren Plateaus in Quantum Convolutional Neural Network. Submitted to *Physical Review X*. (LA-UR-20-29031)

*Roberts, D., L. Cincio, A. Saxena, A. Petukhov and S. Knysh. Noise amplification at spin-glass bottlenecks of quantum annealing: A solvable model. 2020. *Physical Review A*. **101** (4): 042317. (LA-UR-19-28446 DOI: 10.1103/PhysRevA.101.042317)

S. Cerezo de la Roca, M. V., A. Sone, J. Beckey and P. J. Coles. A Generalized Measure of Quantum Fisher Information. Submitted to *Physical Review A*. (LA-UR-20-27870)

S. Cerezo de la Roca, M. V., A. Sone, J. L. Beckey and P. J. Coles. Sub-Quantum Fisher Information. Submitted to *Physical Review Letters*. (LA-UR-21-20536)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, P. J. Czarnik, L. Cincio and P. J. Coles. Effect of barren plateaus on gradient-free optimization. Submitted to *Quantum*. (LA-UR-20-29699)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio and P. J. Coles. Variational Quantum Algorithms. Submitted to *Nature Reviews Physics*. (LA-UR-20-30142)

S. Cerezo de la Roca, M. V., K. Sharma, A. T. Arrasmith and P. J. Coles. Variational Quantum State Eigensolver. Submitted

to *Nature Partner Journal Quantum Information*. (LA-UR-20-22660)

*Sadhukhan, D., A. Sinha, A. Francuz, J. Stefaniak, M. M. Rams, J. Dziarmaga and W. H. Zurek. Sonic horizons and causality in phase transition dynamics. 2020. *Physical Review B*. **101** (14): 144429. (LA-UR-19-30546 DOI: 10.1103/PhysRevB.101.144429)

*Sahinoglu, B. and R. D. Somma. Hamiltonian simulation in the low-energy subspace. 2021. *npj Quantum Information*. **7** (1): 119. (LA-UR-20-23338 DOI: 10.1038/s41534-021-00451-w)

Saxena, A. B., E. G. Charalampidis, F. Cooper, J. F. Dawson and A. Khare. Behavior of solitary waves of coupled nonlinear Schrodinger equations subjected to complex external periodic potentials with anti-PT symmetry. Submitted to *Journal of Physics A*. (LA-UR-20-26645)

Saxena, A. B., F. Cooper, A. Khare, J. F. Dawson and E. G. Charalampidis. Stability of exact solutions of a nonlocal and nonlinear Schrodinger equation with arbitrary nonlinearity. Submitted to *Journal of Physics A*. (LA-UR-21-20590)

Saxena, A. B., F. Cooper and A. Khare. Solitary wave solutions of the 2+1 and 3+1 dimensional nonlinear Dirac equation constrained to planar and space curves. Submitted to *Physics Letters A*. (LA-UR-20-27186)

Saxena, A. B., P. Kumar and A. Khare. A model field theory with (psi log(psi)^2 potential: Kinks with super-exponential profiles. Submitted to *Journal of Physics A*. (LA-UR-19-28140)

Saxena, A. B., Z. A. Cochran and Y. N. Joglekar. Parity-time symmetric systems with memory. Submitted to *Physical Review Research*. (LA-UR-20-27357)

Saxena, A. B. and A. Khare. Novel deformation function creating or destroying any number of even kink solutions. 2021. *Physics Letters A*. 127830. (LA-UR-21-26756 DOI: 10.1016/j.physleta.2021.127830)

Saxena, A. B. and M. Bojowald. From Crystal Color Symmetry to Quantum Spacetime. Submitted to *Acta Crystallographica. Section A: Foundations of Crystallography*. (LA-UR-21-23983)

Schatzki, L., M. V. S. Cerezo de la Roca, A. T. Arrasmith and P. J. Coles. Entangled Datasets for Quantum Machine Learning. Submitted to *Physical Review X Quantum*. (LA-UR-21-28803)

Schmitt, M., M. M. Rams, J. P. Dziarmaga, M. Heyl and W. H. Zurek. Quantum phase transition dynamics in the two-dimensional Ising model. Submitted to *Nature Communications*. (LA-UR-21-24924)

Sharma, K., M. V. S. Cerezo de la Roca, L. Cincio and P. J. Coles. Trainability of Dissipative Perceptron-Based Quantum Neural Networks. Submitted to *Physical Review Letters*. (LA-UR-20-23484)

*Sharma, K., S. Khatri, M. Cerezo and P. J. Coles. Noise resilience of variational quantum compiling. 2020. *New Journal of Physics*. **22** (4): 043006. (LA-UR-19-28095 DOI: 10.1088/1367-2630/ab784c)

*Somma, R. D. Unitary circuit synthesis for tomography of generalized coherent states. 2019. *Journal of Mathematical Physics*. **60** (11): 112202. (LA-UR-18-30016 DOI: 10.1063/1.5121549)

Sone, A., Y. Liu and P. Cappellaro. Quantum Jarzynski equality of open quantum systems in one-time measurement scheme. Submitted to *Physical Review Letters*. (LA-UR-19-32640)

Sone, A. and S. Deffner. Jarzynski equality for conditional stochastic work. Submitted to *Journal of Statistical Physics*. (LA-UR-20-28110)

Sone, A. and S. Deffner. Quantum and classical ergotropy from relative entropies. Submitted to *Physical Review Letters*. (LA-UR-21-22722)

Sornborger, A. T., B. A. Commeau, M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio and P. J. Coles. \xef\xbb\xbfVariational Hamiltonian Diagonalization for Dynamical Quantum Simulation. Submitted to *Quantum*. (LA-UR-20-26827)

Sornborger, A. T., B. A. Commeau, M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio and P. J. Coles. \xef\xbb\xbfVariational Hamiltonian Diagonalization for Dynamical Quantum Simulation. Submitted to *Quantum*. (LA-UR-20-26827)

*Sornborger, A. T., P. J. Coles, L. Cincio, Z. Holmes, C. Cirstoiu and J. T. Iosue. Variational fast forwarding for quantum simulation beyond the coherence time. 2020. *npj Quantum Information*. **6** (1): 82. (LA-UR-19-29521 DOI: 10.1038/s41534-020-00302-0)

*Suba\xc5\x9fı, Y., R. D. Somma and D. Orsucci. Quantum Algorithms for Systems of Linear Equations Inspired by Adiabatic Quantum Computing. 2019. *Physical Review Letters*. **122** (6): 060504. (LA-UR-17-20510 DOI: 10.1103/PhysRevLett.122.060504)

Subasi, Y., K. Sinha and A. E. R. L\xc3\xb3pez. Dissipative dynamics of a particle coupled to field via internal degrees of freedom. Submitted to *Physical Review D*. (LA-UR-21-20103)

*Subasi, Y., L. Cincio and P. J. Coles. Entanglement spectroscopy with a depth-two quantum circuit. 2019. *Journal of Physics A: Mathematical and Theoretical*. **52** (4): 44001. (LA-UR-18-25483 DOI: 10.1088/1751-8121/aaf54d)

*Sun, C., V. Y. Chernyak, A. Piryatinski and N. A. Sinitsyn. Cooperative Light Emission in the Presence of Strong Inhomogeneous Broadening. 2019. *Physical Review Letters*. **123** (12): 123605. (LA-UR-19-25136 DOI: 10.1103/PhysRevLett.123.123605)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. 2022. *Physical Review Letters*. **128** (1): 010401. (LA-UR-21-20437 DOI: 10.1103/PhysRevLett.128.010401)

*Volkoff, T. and P. J. Coles. Large gradients via correlation in random parameterized quantum circuits. 2021. *Quantum Science and Technology*. **6** (2): 025008. (LA-UR-20-23818 DOI: 10.1088/2058-9565/abd891)

*Vyskocil, T. and H. Djidjev. Embedding Equality Constraints of Optimization Problems into a Quantum Annealer. 2019. *Algorithms*. **12** (4): 77. (LA-UR-19-20224 DOI: 10.3390/a12040077)

Wang, S., E. Fontana, M. Cerezo, K. Sharma, A. Sone, L. Cincio and P. J. Coles. Noise-induced barren plateaus in variational quantum algorithms. 2021. *Nature Communications*. **12** (1): 6961. (LA-UR-20-25526 DOI: 10.1038/s41467-021-27045-6)

Wang, S., P. J. Coles, P. J. Czarnik, A. T. Arrasmith, M. V. S. Cerezo de la Roca and L. Cincio. Can Error Mitigation Improve Trainability of Noisy Variational Quantum Algorithms?. Submitted to *Physical Review X, arxiv.org*. (LA-UR-21-28574)

*Xu, Z. and A. Del Campo. Probing the Full Distribution of Many-Body Observables By Single-Qubit Interferometry. 2019. *Physical Review Letters*. **122** (16): 160602. (LA-UR-19-20144 DOI: 10.1103/PhysRevLett.122.160602)

*Yan, B., L. Cincio and W. H. Zurek. Information Scrambling and Loschmidt Echo. 2020. *Physical Review Letters*. **124** (16): 160603. (LA-UR-19-21861 DOI: 10.1103/PhysRevLett.124.160603)

Yan, B., W. Chemissany and W. H. Zurek. Quantum Chaos on Complexity Geometry. Submitted to *Physical Review Letters*. (LA-UR-20-22063)

Yan, B. and N. Sinitsyn. Analytical solution for a general quantum annealing problem. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-21-23292)

Yan, B. and W. H. Zurek. Convolution of decoherence: an interplay between Gaussian and exponential. Submitted to *Physical Review Letters*. (LA-UR-21-28440)

*Yirka, J. and Y. Subasi. Qubit-efficient entanglement spectroscopy using qubit resets. 2021. *Quantum*. **5**: 535. (LA-UR-20-25416 DOI: 10.22331/q-2021-09-02-535)

Zurek, W. H. Quantum jumps, Born's rule, and objective classical reality via quantum Darwinism. Submitted to *Quantum jumps, Born's rule, and objective classical reality via quantum Darwinism*. (LA-UR-19-23643)

Zurek, W. H., A. Touil, B. Yan, D. Girolami and S. Deffner. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Submitted to *Physical Review Letters*. (LA-UR-21-25646)

Conference Papers

Baertschi, A. and S. J. Eidenbenz. Deterministic Preparation of Dicke States. Presented at *22nd International Symposium on Fundamentals of Computation Theory*. (Copenhagen, Denmark, 2019-08-11 - 2019-08-14). (LA-UR-19-22718)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Advanced anneal paths for improved quantum annealing. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Denver, Colorado, United States, 2020-10-12 - 2020-10-12). (LA-UR-20-23828)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Advanced unembedding techniques for quantum annealers. Presented at *IEEE International Conference on Rebooting Computing*. (Virtual Conference, New Mexico, United States, 2020-12-01 - 2020-12-03). (LA-UR-20-26972)

Djidjev, H. N. and T. Vyskocil. Implementing constraints for quantum annealing optimization using finite state automata. Presented at *25th International Computing and Combinatorics Conference (COCOON)*. (Xian, China, 2019-07-29 - 2019-07-29). (LA-UR-19-22730)

Hassan, M. W., S. D. Pakin and W. Feng. C to D-Wave: A High-level C-compilation Framework for Quantum Annealers. Presented at *23rd Annual IEEE High Performance Extreme Computing Conference (HPEC 2019)*. (Waltham, Massachusetts, United States, 2019-09-24 - 2019-09-26). (LA-UR-19-24490)

Khetawat, H., A. Atrey, G. Li, F. Mueller and S. D. Pakin. Implementing NChooseK on IBM Q Quantum Computer Systems. Presented at *11th Conference on Reversible Computation*. (Lausanne, Switzerland, 2019-06-24 - 2019-06-25). (LA-UR-19-23341)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Reducing quantum annealing biases for solving the graph partitioning problem. Presented at *Computing Frontiers 2021 Virtual Conference*. (Catania, Sicily, Italy, 2021-05-11 - 2021-05-13). (LA-UR-21-22206)

Vyskocil, T. and H. N. Djidjev. Constraint embedding for solving optimization problems on quantum annealers. Presented at *21st Workshop on Advances in Parallel and Distributed Computational Models*. (Rio de Janeiro, Brazil, 2019-05-20 - 2019-05-20). (LA-UR-19-21107)

Books/Chapters

Zurek, W. H. Conscious of a Classical World in a Quantum Universe. (LA-UR-20-28307)

Reports

Beckey, J. and A. Sone. Notes on QFI. Unpublished report. (LA-UR-20-28164)

Ch Narayan Chowdhury, A. Quantum Algorithms with Applications to Simulating Physical Systems. Unpublished report. (LA-UR-19-25227)

Cincio, L. Error mitigation with Clifford quantum-circuit data. Unpublished report. (LA-UR-22-21698)

Eidenbenz, S. J., J. Cook and A. Baertschi. The Quantum Alternating Operator Ansatz on Max-k Vertex Cover. Unpublished report. (LA-UR-19-31473)

Pakin, S. D. Unifying Circuit-Model Quantum Computing and Quantum Annealing. Unpublished report. (LA-UR-20-22130)

Pakin, S. D. and F. Mueller. Unifying Circuit-Model Quantum Computing and Quantum Annealing. Unpublished report. (LA-UR-20-22726)

Somma, R. D. and M. B. Sahinoglu. Complexity of product formulas in digital adiabatic state transformations. Unpublished report. (LA-UR-21-23267)

Presentation Slides

Arrasmith, A. T., J. Kubler, L. Cincio, R. D. Somma and P. J. Coles. Shot Frugal Optimization for VQE. Presented at *Quantum Techniques in Machine Learning 2020*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-29153)

Caro, M., H. Huang, M. V. S. Cerezo de la Roca, K. Sharma, L. Cincio and P. J. Coles. Generalization in quantum machine learning from few training data. Presented at *SAMOP21*, Munich, Germany, 2021-09-19 - 2021-09-19. (LA-UR-21-29006)

Ch Narayan Chowdhury, A., R. D. Somma and Y. Subasi. Improved Implementation of Reflection Operators. Presented at *APS March Meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-08. (LA-UR-19-22012)

Cincio, L. Machine learning for quantum computing. Presented at *quantum computing summer school*, Los Alamos, New Mexico, United States, 2020-06-09 - 2020-06-09. (LA-UR-20-24252)

Cincio, L. Variational Quantum Linear Solver. Presented at *Quantum Techniques In Machine Learning 2020*, on-line, New Mexico, United States, 2020-11-09 - 2020-11-12. (LA-UR-20-29266)

Cincio, L. Machine learning of noise-resilient quantum circuits. Presented at *Informs*, on-line, New Mexico, United States, 2021-10-24 - 2021-10-27. (LA-UR-21-28959)

Cincio, L. Quantum Computing School 2021 Outbrief. Presented at *ISTI School Outbrief*, Los Alamos, New Mexico, United States, 2021-09-14 - 2021-09-14. (LA-UR-21-29000)

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Cincio, L., P. J. Coles and M. Sarovar. Machine learning of noise-resilient quantum circuits. Presented at *Quantum Computing User Forum*, Oak Ridge, Tennessee, United States, 2020-04-21 - 2020-04-24. (LA-UR-20-23087)

Cincio, L., S. Thanasilp, V. N. A. Nghiem, S. J. Wang, P. J. Coles and M. V. S. Cerezo de la Roca. Subtleties in the trainability of quantum neural networks. . (LA-UR-21-28118)

Cirstoiu, C., Z. P. Holmes, J. T. Iosue, B. A. Commeau, J. R. Gibbs, K. M. Gili, L. Cincio, P. J. Coles and A. T. Sornborger. Variational Fast Forwarding for NISQ Simulations. Presented at *Quantum Information Processing 2021*, Online, New Mexico, United States, 2021-02-01 - 2021-02-05. (LA-UR-20-29583)

Coles, P. J. Quantum computing in the NISQ era. Presented at *quantum computing summer school*, Los Alamos, New Mexico, United States, 2020-06-09 - 2020-06-09. (LA-UR-20-24251)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Exploiting some advanced annealing options of the D-Wave 2000Q quantum annealer. Presented at *Qubits Worldwide Users Conference*, Virtual Conference, New Mexico, United States, 2020-09-28 - 2020-09-28. (LA-UR-20-27120)

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Parameter optimization for improving quantum annealing accuracy. Presented at *QCE20 Workshop on Tuning Strategies for Quantum Annealing*, Virtual Conference, New Mexico, United States, 2020-10-14 - 2020-10-14. (LA-UR-20-28206)

Kazi, S. S. Studying Dynamical Lie Algebras Generated by Max-Cut Hamiltonian and QAOA Mixer Hamiltonians. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-27740)

Pakin, S. D. May I Have a Real High-Level Quantum Programming Language, Please?. Presented at *SC18 BoF on High-Level Programming Languages for Quantum Computing*, Dallas, Texas, United States, 2018-11-13 - 2018-11-13. (LA-UR-18-30899)

Pakin, S. D. Targeting Classical Code to a Quantum Annealer. Presented at *The 24th ACM International Conference on Architectural Support for Programming Languages and Operating Systems*, Providence, Rhode Island, United States, 2019-04-13 - 2019-04-17. (LA-UR-19-21480)

Pakin, S. D. Targeting Classical Code to a Quantum Annealer. Presented at *24th ACM International Conference on Architectural Support for Programming Languages and Operating Systems*, Providence, Rhode Island, United States, 2019-04-13 - 2019-04-17. (LA-UR-19-23060)

Pakin, S. D. Targeting Classical Code to a Quantum Annealer. Presented at *24th ACM International Conference on Architectural Support for Programming Languages and Operating Systems*, Providence, Rhode Island, United States, 2019-04-13 - 2019-04-17. (LA-UR-19-23407)

Pakin, S. D. Classical Code In, Quantum Code Out. Presented at *Quantum Computing User Forum*, Oak Ridge, Tennessee, United States, 2019-04-24 - 2019-04-25. (LA-UR-19-23650)

Pakin, S. D. Classically Programming a Quantum Annealer. . (LA-UR-19-24190)

Pakin, S. D. Classically Programming a Quantum Annealer. Presented at *2nd IAMCS Workshop on Quantum Computing and Information*, College Station, Texas, United States, 2019-05-13 - 2019-05-15. (LA-UR-19-24336)

Pakin, S. D. Quantum Inspired vs. Quantum Computing—What Next?. Presented at *SC19*, Denver, Colorado, United States, 2019-11-17 - 2019-11-22. (LA-UR-19-31865)

Pakin, S. D. q20_pakin: Quantifying Quantum Processor Fidelity. . (LA-UR-21-21561)

Pakin, S. D., M. W. Hassan and W. Feng. C Code In, D-Wave QMI Out. Presented at *D-Wave Qubits North America Users Conference 2019*, Newport, Rhode Island, United States, 2019-09-23 - 2019-09-25. (LA-UR-19-29334)

Pakin, S. D. and E. G. Rieffel. Introduction to Quantum Computing. Presented at *SC18*, Dallas, Texas, United States, 2018-11-11 - 2018-11-16. (LA-UR-18-29951)

Pakin, S. D. and E. G. Rieffel. Introduction to Quantum Computing. Presented at *SC19*, Denver, Colorado, United States, 2019-11-17 - 2019-11-22. (LA-UR-19-31426)

Pakin, S. D. and M. Strout. Navigating the SC Conference Technical Program Submission Process: Technical Papers. Presented at *SC18*, Dallas, Texas, United States, 2018-11-11 - 2018-11-16. (LA-UR-18-30912)

Saxena, A. B. Quantum Computing at Los Alamos: Algorithms, Error Correction, Hybrid Computing. Presented at *TopQC2019*, Cetraro, Italy, 2019-06-10 - 2019-06-10. (LA-UR-19-25232)

Saxena, A. B. Power-law kink tails in higher order field theories. Presented at *Tsironis Symposium*, Chania, Greece, 2019-06-20 - 2019-06-20. (LA-UR-19-25283)

Sinitsyn, N. Integrable time-dependent quantum Hamiltonians. Presented at *The International Conference dedicated to the 100th anniversary of Isaak Khalatnikov*, Moscow, Russia, 2019-10-16 - 2019-10-22. (LA-UR-19-27585)

Somma, R. D. The Future of Computation. . (LA-UR-18-30625)

Somma, R. D. Quantum computing for quantum field theories. Presented at *Lattice QCD*, Santa Fe, New Mexico, United States, 2019-08-30 - 2019-08-30. (LA-UR-19-28787)

Somma, R. D. Quantum Computing for Condensed Matter. Presented at *QC/QIS for Nuclear Theory*, Santa Fe, New Mexico, United States, 2019-01-23 - 2019-01-23. (LA-UR-19-20419)

Somma, R. D. What is Quantum Computing?. . (LA-UR-19-20444)

Somma, R. D. Hamiltonian Simulation. . (LA-UR-20-23516)

Somma, R. D. Quantum algorithms for systems of linear equations. Presented at *2020 Quantum Summer Symposium*, Los Angeles, California, United States, 2020-07-22 - 2020-07-23. (LA-UR-20-25084)

Somma, R. D. Quantum state verification in the quantum linear systems problem. Presented at *SIAM CSE21*, Fort Worth (online), Texas, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-21863)

Somma, R. D. Quantum computing. Presented at *LANL Quantum Science Workshop*, Los Alamos, New Mexico, United States, 2021-04-19 - 2021-04-19. (LA-UR-21-23670)

Sone, A. Toward understanding work and heat in a quantum system. . (LA-UR-20-25924)

Sone, A. Precision sensing assisted by quantum-classical computation. . (LA-UR-20-27181)

Sone, A. Quantum Jarzynski Equality of Open Quantum Systems. Presented at *Invited talk by Centre for Quantum Dynamics at Griffith University*, Brisbane, Australia, 2020-10-20 - 2020-10-20. (LA-UR-20-28038)

Sone, A., M. V. S. Cerezo de la Roca, J. Beckey and P. J. Coles. Variational Quantum Algorithms for Estimating the Quantum Fisher Information. Presented at *Quantum Science Center, Quantum Algorithms Thrust meeting*, Oak Ridge, Tennessee, United States, 2020-10-28 - 2020-10-28. (LA-UR-20-28687)

Sone, A., Y. Liu and P. Cappellaro. Nonequilibrium work relations of open quantum systems in one-time measurement scheme \xc2\xa0. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21463)

Sone, A. and S. Deffner. Geometry of Thermal States – thermodynamics of quantum and classical coherence. Presented at *March Meeting*, online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-21980)

Sornborger, A. T., B. A. Commeau, M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio and P. J. Coles. Variational Hamiltonian Diagonalization for Dynamical Quantum Simulation. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-19 - 2021-03-19. (LA-UR-21-22530)

Sornborger, A. T., C. Cirstoiu, Z. P. Holmes, J. T. Iosue, B. A. Commeau, K. M. Gili, J. R. Gibbs, L. Cincio and P. J. Coles. Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time. Presented at *IEEE QCE20*, Online, New Mexico, United States, 2020-10-12 - 2020-10-12. (LA-UR-20-27996)

Sornborger, A. T., C. Cirstoiu, Z. P. Holmes, J. T. Iosue, L. Cincio and P. J. Coles. Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time. Presented at *Quantum Computing Forum 2020*, Knoxville, Tennessee, United States, 2020-04-21 - 2020-04-21. (LA-UR-20-23047)

Sornborger, A. T., P. J. Coles, L. Cincio, Z. Holmes, C. Cirstoiu and J. T. Iosue. Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time. Presented at *SQuInT 2020*, Eugene, Oregon, United States, 2020-02-08 - 2020-02-10. (LA-UR-20-21102)

Sornborger, A. T., Z. Holmes, C. Cirstoiu, J. T. Iosue, L. Cincio and P. J. Coles. Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21997)

Subasi, Y. Quantum Linear Systems Problem. . (LA-UR-21-24962)

Subasi, Y., R. D. Somma and N. A. Chowdhury. Computing partition functions in the one clean qubit model. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21758)

Subasi, Y. and J. Jirka. Qubit-efficient entanglement spectroscopy using qubit resets. Presented at *APS March Meeting*, Virtual, Maryland, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22445)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21968)

Posters

Cincio, L., K. Rudinger, M. Sarovar and P. J. Coles. Machine learning of noise-resilient circuits. Presented at *Quantum Algorithms 2020*, Cambridg, online, United Kingdom, 2020-09-22 - 2020-09-22. (LA-UR-20-27368)

Cirstoiu, C., Z. P. Holmes, J. T. Iosue, L. Cincio, P. J. Coles, B. A. Commeau, J. R. Gibbs, K. M. Gili and A. T. Sornborger. Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time. Presented at *QuAlg20*, Oxford, United Kingdom, 2020-09-22 - 2020-09-22. (LA-UR-20-27353)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *QuAlg20*, N/A (virtual), United Kingdom, 2020-09-22 - 2020-09-22. (LA-UR-20-27369)

Sone, A., J. Beckey, M. V. S. Cerezo de la Roca and P. J. Coles. Quantum Fisher information estimation via hybrid quantum-classical computation. Presented at *Quantum Techniques in Machine Learning 2020*, Cambridge, Massachusetts, United States, 2020-11-09 - 2020-11-12. (LA-UR-20-28727)

Subasi, Y. and R. D. Somma. Quantum state verification in the linear systems problem. Presented at *Quantum Imformation Processing (QIP) 2021 Annual Meeting*, Munich, Germany, 2021-02-01 - 2021-02-05. (LA-UR-21-20311)

Other

Sarovar, M. and L. Cincio. Talk given at Quantum Computing Summer School, "Quantum Control: theory and practice". Audio/Visual. (LA-UR-21-28281)

Quantum Computing with Strontium Nuclear Qubits

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Project Description

The subcommittee on Quantum Information Science under the Committee on Science of the National Science and Technology Council published a report in September 2018 entitled "National Strategic Overview for Quantum Information Science." Here, the economic and defense implications of developing a quantum computer are discussed. Cited applications included optimization problems, chemistry, and machine learning. Meanwhile, there is a vast gap between the capabilities of current quantum hardware and the hardware requirements of useful quantum algorithms. For example, chemistry calculations can require qubit numbers of 10,000 to 1,000,000, corresponding to error rates at the part-per-billion to part-per-thousand level, respectively (smaller error rates require fewer qubits). Therefore, an outstanding challenge is to chart a path towards these kinds of performance specifications, the realization of which may be decades in the making. Neutral atom systems, as developed here, are one promising approach. This work will explore a system comprising interacting qubits encoded in the nucleus of the alkaline earth atom strontium, which has already been extensively studied in the field of atomic clocks. The same properties that makes strontium a good atomic clock can also yield good qubits, and we will explore the fundamental interactions and limitations in a few-qubit system.

Publications

Journal Articles

*Mitra, A., M. J. Martin, G. W. Biedermann, A. M. Marino, P. M. Poggi and I. H. Deutsch. Robust M\xc3\xb8lmer-S\xc3\xb8rensen gate for neutral atoms using rapid adiabatic Rydberg dressing. 2020. *Physical Review A*. **101** (3): 030301. (LA-UR-19-31221 DOI: 10.1103/PhysRevA.101.030301)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Optimal Control of Nuclear Spin Qudecimals in 87Sr. Submitted to *Physical Review A*. (LA-UR-21-25988)

Schine, N., A. Young, W. Eckner, M. J. Martin and A. Kaufman. Long-lived Bell states in an array of optical clock qubits. Submitted to *Nature*. (LA-UR-21-29502)

Presentation Slides

Martin, M. J. Quantum information science with Rydberg atoms. . (LA-UR-20-29116)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *UNM CQuIC seminar*, Albuquerque, New Mexico, United States, 2021-02-04 - 2021-02-04. (LA-UR-21-20920)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *LANL/TAMU Quantum Seminar Series*, College Station, Texas, United States, 2021-04-27 - 2021-04-27. (LA-UR-21-23972)

Martin, M. J. Quantum information science and sensing with ultracold neutral atoms. . (LA-UR-21-25997)

Martin, M. J. Quantum information science with laser-dressed atoms Q-SEnSE Convergence Seminar. Presented at *Q-SEnSE Convergence Seminar*, Boulder, Colorado, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32107)

Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

Mitra, A., S. T. Omanakuttan, M. J. Martin, G. W. Biedermann and I. H. Deutsch. Fundamental limits of neutral atom entanglement using Rydberg dressing. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, College Park, Maryland, United States, 2021-05-31 - 2021-06-04. (LA-UR-21-25172)

Omanakuttan, S., A. Mitra, I. H. Deutsch and M. J. Martin. Quantum control of nuclear spins. Presented at *APS Four Corners Meeting*, Albuquerque, New Mexico, United States, 2020-10-23 - 2020-10-24. (LA-UR-20-28577)

Omanakuttan, S., A. Mitra, M. J. Martin and I. Deutsch. Qudit entanglers using quantum control on nuclear-spin qudits. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22133)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Control of Nuclear Spin for Quantum Logic with Qudits. Presented at *APS March Meeting*, College Park, Maryland, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22461)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Control of Nuclear Spin for Quantum Logic with Qudits. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, College Park, Maryland, United States, 2021-05-31 - 2021-06-04. (LA-UR-21-25168)

Posters

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Quantum Optimal Control of Nuclear Spin Qudecimals in 87Sr. Presented at *Q-SEnSE Annual Meeting*, Boulder, Colorado, United States, 2021-07-20 - 2021-07-21. (LA-UR-21-26508)

Omanakuttan, S., A. Mitra, M. J. Martin and I. H. Deutsch. Implementing qudit quantum logic gates on nuclear spins in 87Sr. Presented at *Southwest Quantum Information and Technology Workshop*, Albuquerque, New Mexico, United States, 2021-10-14 - 2021-10-15. (LA-UR-21-30066)

Topological Relation-Based Image Analysis using Graphs

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Project Description

The analysis of technical imagery is critical to matters of national security, including tracking the sharing of technical diagrams for nuclear counterproliferation, quantifying the shapes of components in images of electronics for homeland security, and in quantifying shapes of particles in materials imaging for nuclear forensics. Computer vision, especially through the use of machine learning methods, has dramatically improved the ability to detect objects in images. However, these advances have not yet automated the understanding of information contained in hand-drawn figures, technical diagrams, and imagery produced for scientific inquiry. Our key innovation is the insight that these technical images carry little per pixel information compared with natural images (photographs and video), and that context, topology and shape provide information. By representing images as hierarchical graphs, with annotations on topological relationships, we will model the context and knowledge necessary to perform intelligent analysis of images. We will be able to find altered copies of technical diagrams, whether being shared online or in publications; match tomography images to databases of known commercial electronics; and identify common shapes in materials images for forensics.

Publications

Conference Papers

Bhattarai, M., D. A. Oyen, J. E. Castorena, L. Yang and B. E. Wohlberg. Diagram Image Retrieval using Sketch-Based Deep Learning and Transfer Learning. Presented at *CVPR DIRA Workshop*. (Seattle, Washington, United States, 2020-06-14 - 2020-06-14). (LA-UR-20-22562)

Castorena, J. E., D. A. Oyen and M. Bhattarai. Learning Spatial Relationships between Samples of Image Shapes. Presented at *Conference on Computer Vision and Pattern Recognition*. (Seattle, Washington, United States, 2020-06-14 - 2020-06-19). (LA-UR-20-22517)

Castorena, J. E. and D. A. Oyen. Learning Shapes on Image Sampled Points with Dynamic Graph CNNs. Presented at *IEEE SSIAI 2020*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29). (LA-UR-20-24122)

Gong, M., L. Yang, C. G. Potts, D. A. Oyen, B. E. Wohlberg and V. K. Asari. TGGLines: A Robust Topological Graph Guided Line Segment Detector for Low Quality Binary Images. Presented at *CVPR 2020*. (Seattle, Washington, United States, 2020-06-13 - 2020-06-20). (LA-UR-19-31578)

Gong, M., X. Wei, D. A. Oyen, J. Wu, M. Gryder and L. Yang. Recognizing Figure Labels in Patents. Presented at *AAAI Workshop on Scientific Document Understanding*. (Online, New Mexico, United States, 2021-02-02 - 2021-02-02). (LA-UR-20-29690)

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval. Presented at *Winter Application on Computer Vision*. (Waikoloa, Hawaii, United States, 2022-01-04 - 2022-01-08). (LA-UR-21-28183)

Kucer, M. and D. A. Oyen. DeepPatent: large scale patent image recognition and retrieval. Presented at *Computer Vision and Pattern Recognition (CVPR) 2021*. (Virtual, New Mexico, United States, 2021-06-19 - 2021-06-19). (LA-UR-20-29372)

Kucer, M. and D. A. Oyen. DeepPatent: Large scale patent image recognition and retrieval. Presented at *International Conference on Computer Vision 2021*. (Montreal, Canada, 2021-10-10 - 2021-10-17). (LA-UR-21-22455)

Kucer, M. and D. A. Oyen. Transfer Learning with fewer ImageNet classes. Presented at *021 Conference on Neural Information Processing Systems*. (Sydney, Australia, 2021-12-06 - 2021-12-14). (LA-UR-21-29446)

Oyen, D. A., M. Kucer and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *SPIE Conference on Machine Learning*. (San Diego, California, United States, 2021-08-03 - 2021-08-03). (LA-UR-21-27432)

Oyen, D. A., M. L. Dubey and M. Kucer. Duplicate Image Detection for Fast Identification of Easily-Confused Classes in ImageNet. Presented at *NeurIPS Workshop on ImageNet*. (Virtual, New Mexico, United States, 2021-12-13 - 2021-12-13). (LA-UR-21-29269)

Oyen, D. A. and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented

at *Workshop on Applications of Computer Vision*. (Virtual, New Mexico, United States, 2021-01-05 - 2021-01-05). (LA-UR-20-27837)

Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodama, D. Bouchez and M. Uyttewaal. Diff2Dist: Differentiable Graph Diffusion Distance. Presented at *The Sixth International Workshop on Deep Learning on Graphs: Methods and Applications*. (Singapore, Singapore, 2021-08-14 - 2021-08-14). (LA-UR-21-24905)

Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodera, M. Uyttewaal and D. Boucher. Diff2Dist: Learning Spectrally Distinct Edge Functions, with Applications to Cell Morphology Analysis. Presented at *German Conference on Pattern Recognition*. (Online, Germany, 2021-09-28 - 2021-09-28). (LA-UR-21-25927)

Presentation Slides

Bhattarai, M., D. A. Oyen, J. E. Castorena, L. Yang and B. E. Wohlberg. Diagram Image Retrieval using Sketch-Based Deep Learning and Transfer Learning. Presented at *Diagram Image Retrieval and Analysis (DIRA): Representation, Learning, and Similarity Metrics*, Seattle, Washington, United States, 2020-06-14 - 2020-06-16. (LA-UR-20-23817)

Castorena, J. E., D. A. Oyen and M. Bhattarai. Learning Spatial Relationships between Samples of Patent Image Shapes. Presented at *IEEE Computer Vision and Pattern Recognition*, Seattle, Washington, United States, 2020-06-14 - 2020-06-14. (LA-UR-20-24123)

Castorena, J. E. and D. A. Oyen. Learning Shapes on Image Sampled Points with Dynamic Graph CNNs. Presented at *2020 IEEE Southwest Symposium on Image Analysis and Interpretation*, Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29. (LA-UR-20-24124)

Gong, M., X. Wei, D. A. Oyen, J. Wu, M. Gryder and L. Yang. Recognizing Figure Labels in Patents. Presented at *AAAI Workshop on Scientific Document Understanding*, Online, New Mexico, United States, 2021-02-09 - 2021-02-09. (LA-UR-21-21174)

U. Hoque, M. R., D. A. Oyen and J. Wu. Segmenting Technical Drawing Figures in US Patents. Presented at *LANL Student Symposium*, Virtual, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27599)

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval. Presented at *Winter Application on Computer Vision 2022*, Waikoloa, Hawaii, United States, 2022-01-04 - 2022-01-08. (LA-UR-21-32274)

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval - dataset and a trained model. Presented at *WACV*, Waikoloa, Hawaii, United States, 2022-01-03 - 2021-12-08. (LA-UR-21-32339)

Oyen, D. A. Image Signatures for Diagram Image Retrieval. Presented at *Southwest Symposium on Image Analysis and Interpretation*, Santa Fe, New Mexico, United States, 2020-03-30 - 2020-03-30. (LA-UR-20-22595)

Oyen, D. A., J. E. Castorena, B. E. Wohlberg, L. Yang, M. Gong, C. Potts and M. Bhattarai. GoFigure: Tracking the Dissemination of Technical Information in Images. Presented at *DHS Science and Technology Symposium*, Washington, District Of Columbia, United States, 2020-07-13 - 2020-07-13. (LA-UR-20-25121)

Oyen, D. A., M. Kucer and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *SPIE Machine Learning*, San Diego, California, United States, 2021-08-01 - 2021-08-01. (LA-UR-21-26622)

Oyen, D. A., M. Kucer and B. E. Wohlberg. VisHash: Visual Similarity Preserving Image Hashing for Diagram Retrieval. Presented at *SPIE Machine Learning*, San Diego, California, United States, 2021-08-01 - 2021-08-01. (LA-UR-21-26662)

Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodera, D. Bouchez and M. Uttyewaal. Diff2Dist: Differentiable Graph Diffusion Distance. Presented at *Knowledge Discovery and Data Mining*, Virtual, New Mexico, United States, 2021-08-14 - 2021-08-14. (LA-UR-21-27979)

Posters

Kucer, M., D. A. Oyen, J. E. Castorena and J. Wu. DeepPatent: Large scale patent drawing recognition and retrieval. Presented at *Winter Application on Computer Vision 2022*, Waikoloa, Hawaii, United States, 2022-01-04 - 2022-01-08. (LA-UR-21-31913)

Adaptive High-order Finite Element Arbitrary Lagrangian-Eulerian (ALE) Methods for Multi-material Hydrodynamics

Jacob Waltz
20200201ER

Project Description

This research improves the accuracy, fidelity, and efficiency of, and therefore increases our trust in, the numerical simulation of multi-material hydrodynamics, which is a critical ingredient of multiple Laboratory/ Department of Energy (DOE) and National Nuclear Security Administration (NNSA) programs. This work will establish the applicability of a heretofore unexplored combination of modern and adaptive numerical methods for multi-material problems combined with automatic load balancing that also enables efficient use of supercomputing hardware. This project also addresses multiple shortcomings in the current state of-practice by using modern numerical methods, previously unexplored in the context of multi-material flows at Los Alamos National Laboratory, in academia, or industry.

Publications

Journal Articles

Li, W., A. K. Pandare, H. Luo, J. Bakosi and J. I. Waltz. A Parallel p-adaptive Discontinuous Galerkin Method for the Euler Equations with Dynamic Load-Balancing on Tetrahedral Grids. Submitted to *Computers & Fluids*. (LA-UR-21-24430)

*Pandare, A. K., J. Waltz and J. Bakosi. Multi-material hydrodynamics with algebraic sharp interface capturing. 2021. *Computers & Fluids*. **215**: 104804. (LA-UR-20-25462 DOI: 10.1016/j.compfluid.2020.104804)

Conference Papers

Li, W., H. Luo, A. K. Pandare and J. Bakosi. A p-adaptive Discontinuous Galerkin Methods for Compressible Flows Using CHARM++. Presented at *AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-20-27898)

Pandare, A. K., J. I. Waltz and J. Bakosi. A Discontinuous Galerkin method for Non-Equilibrium Multi-Material Flows on Unstructured Grids. Presented at *AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-32156)

Pandare, A. K., J. I. Waltz and J. Bakosi. Algebraic sharp interface capturing for non-equilibrium multi-material flows. Presented at *AIAA SciTech 2021 Forum*. (Nashville, Tennessee, United States, 2021-01-11 - 2021-01-21). (LA-UR-20-29614)

Pandare, A. K., W. Li, J. I. Waltz, J. Bakosi and H. Luo. A THINC-DG Method for Multi-Material Fluid Flow. Presented at *AIAA SciTech Forum 2022*. (San Diego, California, United States, 2022-01-03 - 2022-01-07). (LA-UR-21-31586)

Presentation Slides

Pandare, A. K., J. I. Waltz and J. Bakosi. A DG Method for Non-Equilibrium Multi-Material Flows on Unstructured Grids. Presented at *AIAA SciTech Forum 2020*, Orlando, Florida, United States, 2020-01-06 - 2020-01-10. (LA-UR-20-20119)

Pandare, A. K., J. I. Waltz and J. Bakosi. Algebraic sharp interface capturing for non-equilibrium multi-material flows. Presented at *AIAA SciTech 2021 Forum*, Nashville, Tennessee, United States, 2021-01-11 - 2021-01-11. (LA-UR-20-29855)

Pandare, A. K., W. Li, J. I. Waltz, J. Bakosi and H. Luo. A THINC-DG Method for Multi-Material Flow. Presented at *AIAA Scitech 2022 Forun*, san diego, California, United States, 2022-01-03 - 2022-01-03. (LA-UR-21-31796)

Waltz, J. I., A. K. Pandare, J. Bakosi, W. Li and H. Luo. Adaptive high-order finite element ALE methods for multi-material hydrodynamics. . (LA-UR-21-23483)

Sampling the Unknown: Robust Modeling of Atomic Potentials

Kipton Barros
20200209ER

Project Description

Machine Learning (ML) is revolutionizing the field of interatomic potential development. If successful, this project will produce a collection of methodologies for fully automated development of ML-based interatomic potentials, with robust density functional theory (DFT)-level accuracies and transferability to a broad range of physical processes. The cost of our force calculations scales linearly with system size, and the prefactor is about 100x that of classical potentials. At the end of this project, we anticipate that our distributed and graphics processing unit (GPU)-optimized ML codes will enable the simulation of millions of atoms with DFT-level accuracy.

Publications

Journal Articles

Barros, K. M., M. Shahzad and S. H. Curnoe. Phase Diagram of a Spin-ice Kondo Lattice Model in the Breathing Pyrochlore Lattice. Submitted to *Physical Review B*. (LA-UR-20-25625)

*Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. 2020. *The Journal of Chemical Physics*. **153** (10): 104502. (LA-UR-19-31421 DOI: 10.1063/5.0017894)

*Craven, G. T., N. Lubbers, K. Barros and S. Tretiak. Determination of Structural Correlation Functions. 2020. *The Journal of Physical Chemistry Letters*. **11** (11): 4372-4378. (LA-UR-19-32446 DOI: 10.1021/acs.jpclett.0c00627)

Gao, X., F. Ramezanghorbani, J. S. Smith and A. E. Roitberg. TorchANI: A Free and Open Source PyTorch Based Deep Learning Implementation of the ANI Neural Network Potentials. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22710)

Gupta, P. L., J. S. Smith and A. E. Roitberg. Rationalizing the pH-activity response of Escherichia coli glycinamide ribonucleotide transformylase through computational methods. Submitted to *Journal of Physical Chemistry B*. (LA-UR-21-21573)

Kulichenko, M., J. S. Smith, B. T. Nebgen, N. S. Fedik, N. E. Lubbers, Y. W. Li, K. M. Barros, A. I. Boldyrev and S. Tretiak. The rise of data science for materials and chemical dynamics. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-23254)

Sifain, A. E., L. A. Lystrom, R. A. Messerly, J. S. Smith, B. T. Nebgen, K. M. Barros, S. Tretiak, N. E. Lubbers and B. J. Gifford. Predicting Phosphorescence and Inferring Wavefunction Localization with Machine Learning. Submitted to *Chemical Science*. (LA-UR-21-21632)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, H. A. Nam, T. C. Germann, S. J. Fensin and K. M. Barros. Automated discovery of a robust interatomic potential for aluminum. Submitted to *Nature Communications*. (LA-UR-20-22194)

Smith, J. S., C. Devereux, K. K. Davis, R. Zubatyuk, K. M. Barros, O. Isayev and A. E. Roitberg. Extending the applicability of the ANI deep learning molecular potential to Sulfur and Halogens. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-20841)

Smith, J. S., N. E. Lubbers, A. P. Thompson and K. M. Barros. Simple and efficient algorithms for training machine learning potentials to force data. Submitted to *Journal of Chemical Physics*. (LA-UR-20-24120)

Wu, X., S. Wen, H. Song, T. Frauenheim, S. Tretiak, C. Yam and Y. Zhang. Nonadiabatic Molecular Dynamics Simulations Based on Time-Dependent Density Functional Tight-Binding Method. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-32095)

Presentation Slides

Barros, K. M. Discovering Robust Inter-Atomic Potentials with Active Learning. Presented at *Telluride workshop*, Los Alamos, New Mexico, United States, 2020-07-28 - 2020-07-28. (LA-UR-20-25626)

Barros, K. M. Discovering Robust Inter-Atomic Potentials with Active Learning. Presented at *Southern California Hub Workshop*, Irvine, California, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28294)

Barros, K. M. Using machine learning to build robust interatomic potentials for bulk metals. Presented at *Machine Learning in Chemical and Materials Sciences*,

Los Alamos, New Mexico, United States, 2021-05-13 - 2021-05-13. (LA-UR-21-24661)

Barros, K. M., S. J. Fensin, B. T. Nebgen, J. S. Smith, N. E. Lubbers, S. Tretiak, T. C. Germann and N. Mathew. Building surrogate models for interatomic potentials. Presented at *Simulations and computations of multiscale and out of equilibrium phenomena*, Los Alamos, New Mexico, United States, 2022-03-09 - 2022-03-10. (LA-UR-22-22233)

Barros, K. M. and J. S. Smith. Midterm LDRD Appraisal 20200209ER. . (LA-UR-20-29553)

Dahlbom, D. A., K. M. Barros and Y. W. Li. Fast Langevin Spin Dynamics on Many GPUs. . (LA-UR-21-27534)

Kulichenko, M., J. S. Smith, K. M. Barros and S. Tretiak. Diversification of ML datasets via "uncertainty" as a bias potential. Presented at *American Chemical Socienty Spring 2021*, Logan, Utah, United States, 2021-04-05 - 2021-04-30. (LA-UR-21-23523)

Makos, M. Z., R. B. Jadrich, E. Kraka, K. M. Barros, N. E. Lubbers and J. S. Smith. ML-based nano-reactor potential via active learning. Presented at *PASC21 Conference*, Geneva, Switzerland, 2021-07-05 - 2021-07-09. (LA-UR-21-26201)

Matin, S., M. S. Wilson, X. Bai, K. M. Barros, Y. W. Li, C. Miles, D. Brooks, M. Mourigal, C. D. Batista, H. Zhang and D. A. Dahlbom. Efficient Inference of Hamiltonian Parameters using Bayesian Optimization. Presented at *CSP Workshop, University of Georgia*, Online, New Mexico, United States, 2022-02-21 - 2022-02-21. (LA-UR-22-21827)

Sattar, N. S. and Y. W. Li. Accelerating parallel Monte Carlo simulations for statistical physics: Portability on many-core processors. Presented at *Parallel Computing Summer Research Internship Student Presentation*, Los Alamos, New Mexico, United States, 2021-08-05 - 2021-08-05. (LA-UR-21-27479)

Smith, J. S. Robust atomistic potentials from machine learning. . (LA-UR-21-23605)

Smith, J. S., K. M. Barros, S. Tretiak, N. Mathew, B. T. Nebgen, J. Chen, S. J. Fensin, T. C. Germann and N. E. Lubbers. Automated discovery of a robust interatomic potential for aluminum. Presented at *Arizona Days*, Pheonix, Arizona, United States, 2020-05-19 - 2020-05-19. (LA-UR-20-23703)

Smith, J. S., S. Tretiak, K. M. Barros, B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, S. J. Fensin, T. C. Germann, O. Isayev, A. E. Roitberg and R. Zubatyuk. Robust atomistic potentials from machine learning. . (LA-UR-19-31336)

Other

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, H. A. Nam, T. C. Germann, S. J. Fensin and K. M. Barros. Training dataset and model parameters for: "Automated discovery of a robust interatomic potential for aluminum". Dataset. (LA-UR-20-27198)

Unlocking the Power of Tensor Cores with Mixed Precision Algorithms

Anders Niklasson
20200225ER

Project Description

The world's most powerful computer, Summit at Oak Ridge National Laboratory, is currently rated at 144 petaflops, but it would exceed 4 exaflops only with its tensor core units if they only could be fully utilized for some general science application. This is currently not the case, since the tensor cores are highly specialized with a peak performance optimized for machine learning with convolutional deep neural networks using half-precision floating point operations. The goal of this project is the development of mixed precision algorithms that can harness the unprecedented power of tensor cores for more general real-world science applications, including electronic structure calculations and quantum-based molecular dynamics simulations. This would potentially extend accessible, predictive, simulation capabilities in time or length scale of materials systems by up to two-orders of magnitude compared to current methods. Our project will help maintain United States leadership in advanced scientific computing and directly support ongoing exascale research projects.

Publications

Journal Articles

Finkelstein, J. D., E. H. Rubensson, S. M. Mniszewski, C. F. A. Negre and A. M. Niklasson. Quantum perturbation theory using tensor cores and a deep neural network. Submitted to *Journal of Chemical Physics*. (LA-UR-22-21647)

Finkelstein, J. D., J. S. Smith, S. M. Mniszewski, K. M. Barros, C. F. A. Negre, E. H. Rubensson and A. M. Niklasson. Mixed Precision Fermi-Operator Expansion on Tensor Cores from a Machine Learning Perspective. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-20350)

Finkelstein, J., J. S. Smith, S. M. Mniszewski, K. Barros, C. F. A. Negre, E. H. Rubensson and A. M. N. Niklasson. Quantum-Based Molecular Dynamics Simulations Using Tensor Cores. 2021. *Journal of Chemical Theory and Computation*. **17** (10): 6180-6192. (LA-UR-21-25427 DOI: 10.1021/acs.jctc.1c00726)

Presentation Slides

Finkelstein, J. D. Quantum-based Molecular Dynamics with Tensor Cores. . (LA-UR-21-25428)

Niklasson, A. M. Unlocking the Power of Tensor Cores with Mixed Precision Algorithms. Presented at *Informal zoom meeting with google sandbox team*, Los Alamos, New Mexico, United States, 2021-04-26 - 2021-04-26. (LA-UR-21-23932)

Niklasson, A. M. Unlocking the Power of Tensor Cores with Mixed Precision Algorithms, LANL Project Overview. . (LA-UR-22-22232)

Dielectric Antenna Array for Pinpoint Data/Energy Targeting

John Singleton
20200285ER

Project Description

This project designs, constructs and tests a new type of radio transmitter that focuses a signal so that it is easily understood at an intended target but scrambled in other places. The transmitter comprises an array of special dielectric antennas developed at Los Alamos National Laboratory. In these antennas, the emission of radio waves is due to moving polarization currents that travel faster than the speed of light in a vacuum, and which are distributed throughout the whole dielectric. These antennas can be built in unusual shapes (flat panels, cylinders, disks), optimized to particular situations and could form part of the ceramic armor applied to future armored vehicles. The outcome represents a fundamental shift in wireless battlefield communications. For over a hundred years procedures have hardly changed; signals are broadcast with little or no directivity, selectivity of reception being via the use of one or more narrow frequency bands. These methods are vulnerable to interception and jamming. In place of this, our technology employs a spread of frequencies to transmit information to a precise location. Decoding/jamming the signal elsewhere is much harder, especially in the context of a rapidly changing conflict situation where transmitter and target are moving.

Publications

Journal Articles

Schmidt, A. C. and J. Singleton. Fatal flaws in the theory of electromagnetic radiation that disobeys the inverse-square law: mathematical and physical considerations. Submitted to *Journal of Plasma Physics*. (LA-UR-20-23586)

Schmidt, A. C. and J. Singleton. Electromagnetic radiation from a polarization current in circular faster-than-light motion; theory and an experimentally realized example. Submitted to *Journal of Plasma Physics*. (LA-UR-21-30110)

*Singleton, J., A. C. Schmidt, C. Bailey, J. Wigger and F. Krawczyk. Information Carried by Electromagnetic Radiation Launched from Accelerated Polarization Currents. 2020. *Physical Review Applied*. **14** (6): 064046. (LA-UR-20-23902 DOI: 10.1103/ PhysRevApplied.14.064046)

Singleton, J. and A. C. Schmidt. Launching information from faster-than-light polarization currents. Submitted to *Research Features*. (LA-UR-21-30356)

Presentation Slides

Schmidt, A. C. and J. Singleton. Meet the Lightslingers. . (LA-UR-22-20640)

Accelerating Combinatorial Optimization with Noisy Analog Hardware

Carleton Coffrin
20210114ER

Project Description

The slowing advance of traditional digital computing hardware has spurred a renaissance in analog computing platforms, which are dedicated to performing specialized computational tasks. This work will help Los Alamos National Laboratory (LANL) scientists develop a deeper understanding of what computational benefits these analog computing platforms can provide. This understanding is a critical first step to integrating analog computing platforms into mission critical computational tasks conducted at LANL for the Department of Energy/ National Nuclear Security Administration.

Publications

Journal Articles

Nelson, J., M. Vuffray, A. Y. Lokhov and C. C. Coffrin. Single-Qubit Fidelity Assessment of Quantum Annealing Hardware. 2021. *IEEE Transactions on Quantum Engineering*. **2**: 3102310. (LA-UR-21-23013 DOI: 10.1109/TQE.2021.3092710)

Vuffray, M. D., C. J. Coffrin, Y. A. Kharkov and A. Lokhov. Programmable Quantum Annealers as Noisy Gibbs Samplers. Submitted to *Science*. (LA-UR-20-28047)

Reports

Coffrin, C. J. Harnessing the Potential of Heterogeneous Computing with Declarative Programming and Artificial Intelligence. Unpublished report. (LA-UR-22-20249)

Nelson, J. A., M. D. Vuffray, A. Lokhov, T. Albash and C. J. Coffrin. High-quality Thermal Gibbs Sampling with Quantum Annealing Hardware. Unpublished report. (LA-UR-21-28692)

Suau, A., J. A. Nelson, M. D. Vuffray, A. Lokhov, L. Cincio and C. J. Coffrin. Single-Qubit Cross Platform Comparison of Quantum Computing Hardware. Unpublished report. (LA-UR-21-28409)

Presentation Slides

Coffrin, C. J. Reflections on Benchmarking of Quantum Accelerated Optimization. . (LA-UR-21-30662)

Coffrin, C. J., Y. Pang, A. Lokhov and M. D. Vuffray. Benchmarking Ising Model Optimization with Corrupted Biased Ferromagnets. Presented at *Adiabatic Quantum Computing 2021*, Tokoy, Japan, 2021-06-22 - 2021-06-25. (LA-UR-21-25773)

Nelson, J. A., M. D. Vuffray, A. Lokhov and C. J. Coffrin. Single Qubit Fidelity Assessment of Quantum Annealing Hardware. Presented at *Adiabatic Quantum Computing 2021*, Tokyo, Japan, 2021-06-22 - 2021-06-25. (LA-UR-21-25778)

Vuffray, M. D., C. J. Coffrin, Y. Kharkov and A. Lokhov. Programmable Quantum Annealers as Noisy Gibbs Samplers. Presented at *Adiabatic Quantum Comouting Conference (AQC) 2021*, Tokyo, Japan, 2021-06-22 - 2021-06-25. (LA-UR-21-25991)

Other

Nagarajan, H., O. Lockwood and C. J. Coffrin. QuantumCircuitOpt: An Open-source Framework for Provably Optimal Quantum Circuit Design. Audio/Visual. (LA-UR-21-31731)

Strategies for Topological Quantum Computing with Braiding of Vortices and Skyrmions

Charles Reichhardt
20210269ER

Project Description

Quantum computing utilizes the properties of quantum mechanics to perform certain computations much more rapidly than a classical computer and to solve problems that are entirely beyond their reach. Realizing quantum computing will have enormous implications for national security, economic, and scientific advances. Department of Energy (DOE) and Los Alamos National Laboratory (LANL) have identified quantum computing as an area of concentration. Topological quantum computers (TQC) bypass the problem of short qubit decoherence times and logical errors by harnessing topologically protected qubits made from quasiparticles such as Majorana Fermions (MFs), but robust methods for manipulating the MFs to form quantum logic gates are still lacking. This project uses superconducting vortices and magnetic skyrmions that are stabilized by a periodic pinning array and manipulated with scanning tips or bulk currents to realize the logic operations needed for a physical realization of a TQC. We will identify the most efficient logic gate designs based on our novel concept and will work with external experimental groups who can test and verify the logic gate operations. If successful, this work will pave the way towards the construction of the first practical, scalable TQC device, placing LANL at the forefront of quantum computing.

Publications

Journal Articles

Reichhardt, C. J., C. Reichhardt, B. Janko and L. Wenzhao. Vortex Ordering and Dynamics of Santa Fe Artificial Ice Pinning Arrays. Submitted to *Applied Physics Letters*. (LA-UR-21-20715)

Reichhardt, C. J. and C. Reichhardt. Statistical Mechanics: The Exceptional Point Proves the Rule. Submitted to *Nature*. (LA-UR-21-22471)

Reichhardt, C., C. J. Reichhardt, A. Duzgun and C. Nisoli. Directed motion of liquid crystal skyrmions with oscillating fields.. Submitted to *New Journal of Physics*. (LA-UR-21-31943)

Reichhardt, C., C. J. Reichhardt, B. Janko and W. Li. Vortex Dynamics, Pinning and Magic Angles on Moire Patterns. Submitted to *Physical Review Letters*. (LA-UR-20-30327)

Reichhardt, C., C. J. Reichhardt, E. J. Roe and M. Eskildsen. Driven vortex dynamics in systems with two-fold anisotropy in the presence of pinning. Submitted to *New Journal of Physics*. (LA-UR-22-21806)

Reichhardt, C., C. J. Reichhardt, F. Yan, L. Wei and M. Murrillo. Structure and dynamical properties of two-dimensional dusty plasmas on one-dimensional periodic substrates. Submitted to *Physics of Plasmas*. (LA-UR-21-20302)

Reichhardt, C., C. J. Reichhardt, L. Varga and A. Libal. Active Phases for Particles on Resource Landscapes. Submitted to *Physical Review Letters*. (LA-UR-21-28307)

Reichhardt, C., C. J. Reichhardt, N. Vizarim, J. Bellizotti Souza, P. Venehas and M. Milosevic. Soliton Motion in Skyrmion Chains. Submitted to *Physical Review B*. (LA-UR-22-21498)

Reichhardt, C., C. J. Reichhardt, N. Vizarim, J. Bellizotti Souza and P. Venegas. Directional Locking ad the Influence of Obstacle Density on Skyrmion Dynamics in Triangular and Honeycomb Arrays.. Submitted to *Journal of Physics: Condensed Matter*. (LA-UR-21-22422)

Reichhardt, C., C. J. Reichhardt, S. Bellizotti, B. Vizarim and P. Venegas. Skyrmion Ratchet in Funnel Geometries. Submitted to *Physical Review B*. (LA-UR-21-24719)

Reichhardt, C., C. J. Reichhardt, Y. Huang, W. Li and Y. Feng. Phonon spectra of a two-dimensional solid dusty plasma modified by two-dimensional periodic substrates. Submitted to *European Physical Journal E. Soft Matter*. (LA-UR-21-28922)

Reichhardt, C., C. J. Reichhardt and A. del Campo. Kibble-Zurek Mechanism for Nonequilibrium Physics Transitions in Driven Systems with Quenched DIsdoer. Submitted to *Nature Communications*. (LA-UR-22-21651)

Reichhardt, C., C. J. Reichhardt and M. Milosevic. Statics and Dynamics of Skyrmions Interacting with Pinning: A Review. Submitted to *Reviews of Modern Physics*. (LA-UR-21-21628)

Reichhardt, C. and C. J. Reichhardt. Drive dependence of the Hall Angle for a sliding Wigner crystal in a magnetic field. Submitted to *Physical Review B*. (LA-UR-20-29718)

Reichhardt, C. and C. J. Reichhardt. Dynamics and Nonmonotonic Drag for Individually Driven Skyrmions. Submitted to *Physical Review B*. (LA-UR-21-25393)

Reichhardt, C. and C. J. Reichhardt. Active Rheology in Odd Viscosity Systems. Submitted to *Europhysics Letters*. (LA-UR-21-25453)

Reichhardt, C. and C. J. Reichhardt. Fluctuations and pinning for individually manipulated skyrmions. Submitted to *Frontiers in Physics*. (LA-UR-21-28609)

Reichhardt, C. and C. J. Reichhardt. Active rheology and anti-commensuration effects for driven probe particles on two dimensional periodic pinning substrates. Submitted to *Physical Review Research*. (LA-UR-21-32117)

Reichhardt, C. and C. J. Reichhardt. Commensuration Effects on Skyrmion Hall Angle and Drag For Manipulation of Skyrmions on Two-Dimensional Periodic Substates. Submitted to *Physical Review B*. (LA-UR-22-20879)

Reichhardt, C. and C. J. Reichhardt. Reversible to Irreversible Transitions For Cyclical Driven Particles on Periodic Obstacle Arrays. Submitted to *Journal of Chemical Physics*. (LA-UR-22-21187)

Saglam, H., C. Nisoli, P. Schiffer and A. Duzgun. Entropy-driven order in an array of nanomagnets. Submitted to *Nature Physics*. (LA-UR-22-21456)

Presentation Slides

Duzgun, A. and A. B. Saxena. Interaction of tilted liquid crystal skyrmions. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22660)

Reichhardt, C. J. and C. Reichhardt. Clogging Dynamics of Active and Passive Disks in Complex Environments. Presented at *APS March Meeting*, Virtual, Tennessee, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22534)

Deep Learning in a Noisy World: Algorithms for Robust Training and Predictive Uncertainty

Sunil Thulasidasan
20210356ER

Project Description

Machine learning using deep neural networks – also called "Deep Learning" (DL) - has been at the center of practically every major advance in artificial intelligence over the last several years and there is now tremendous interest in using DL-based systems in all domains where computers can be used to make predictions after being trained on large quantities of data. The proposed work will develop algorithms to overcome two significant challenges when using DL for mission applications. 1. State-of-the-art Deep Neural Networks (DNNs) -- that form the core of the deep learning pipeline -- need to be trained on large amounts of clean, well-labeled data, which is often infeasible in the real world where noisy data is the norm. 2. Trained DNNs are unable to provide reliable estimates of predictive uncertainty, a crucial need in mission space. Standard training techniques result in over-confident predictions, especially when presented with data from categories not seen during training. That is, standard deep models "do not know what they don't know". The proposed effort will build on recent fundamental advances by our team in these areas to develop a broadly applicable, general-purpose framework for improving robustness and predictive uncertainty in deep learning.

Publications

Journal Articles

Porter, R. B., B. G. Zimmer, Q. Nguyen and V. Jatla. End-to-End Learning of Hierarchical Watersheds. Submitted to *Journal of Mathematical Imaging and Vision*. (LA-UR-21-20143)

Conference Papers

Singh, H. S. Synthetic-to-Real Domain Adaptation for Autonomous Driving. Presented at *Smoky Mountains Challenge*. (Oak Ridge, Tennessee, United States, 2021-10-18 - 2021-10-18). (LA-UR-21-30388)

Thulasidasan, S., S. Thapa, S. Dhaubhadel, G. Chennupati, T. Bhattacharya and J. Bilmes. An Effective Baseline for Robustness to Distributional Shift. Presented at *20th IEEE INTERNATIONAL CONFERENCE ON MACHINE LEARNING AND APPLICATIONS*. (Pasadena, California, United States, 2021-12-13 - 2021-12-16). (LA-UR-21-30506)

Reports

Pang, X., S. Thulasidasan and L. J. Rybarcyk. Autonomous Control of a Particle Accelerator using Deep Reinforcement Learning. Unpublished report. (LA-UR-20-28238)

Thulasidasan, S., A. A. Jivan, T. Bhattacharya, G. Chennupati and J. Bilmes. A Control-Theoretic Approach to Robust Learning in the Presence of Label Noise. Unpublished report. (LA-UR-21-30505)

Posters

Singh, H. S. Synthetic-to-Real Domain Adaptation for Autonomous Driving. Presented at *SMC Data Challenge 2021*, Oak Ridge, Tennessee, United States, 2021-10-18 - 2021-10-18. (LA-UR-21-30163)

Unifying Circuit-Model Quantum Computing and Quantum Annealing

Scott Pakin
20210397ER

Project Description

In the stockpile-stewardship arena, national security is largely dependent on who can out-compute whom. This is why all the National Nuclear Security Administration (NNSA) laboratories and other government national-security groups have traditionally invested so heavily in state-of-the-art supercomputers. It is also why quantum computing is now so appealing. For certain problems, it is believed that a single quantum computer will one day outperform all of the world's conventional computers combined. Alas, quantum programming not only exhibits virtually no traits in common with classical programming but is extremely challenging. Forthcoming quantum hardware with large computational abilities offers little benefit if only a small number of quantum-computing experts are able to program such devices. This project addresses the programmability problem by attempting to define and implement a new programming model that is relatively easy for non-experts in quantum computing to learn and that can be implemented—with varying performance characteristics—on different types of quantum (and classical) computers with little or no modification to programs. If successful, when high-performance quantum computers are finally available, programmers and computational scientists in national-security areas will be able to take advantage of them.

Publications

Conference Papers

Pakin, S. D. A Simple Heuristic for Expressing a Truth Table as a Quadratic Pseudo-Boolean Function. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Online, New Mexico, United States, 2021-10-18 - 2021-10-22). (LA-UR-21-25343)

Wilson, E., F. Mueller and S. D. Pakin. Mapping Constraint Problems onto Quantum Gate and Annealing Devices. Presented at *2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS)*. (St. Louis, Missouri, United States, 2021-11-15 - 2021-11-15). (LA-UR-21-30718)

Presentation Slides

Pakin, S. D. Running Classical Programs on a Quantum Annealer. . (LA-UR-21-23768)

Pakin, S. D. A Simple Heuristic for Expressing a Truth Table as a Quadratic Pseudo-Boolean Function. Presented at *IEEE International Conference on Quantum Computing and Engineering (QCE 21)*, Online, New Mexico, United States, 2021-10-17 - 2021-10-22. (LA-UR-21-29644)

Pakin, S. D. Running a Quantum Annealer in an HPC Data Center. Presented at *First International Workshop on Integrating High-Performance Computing with Quantum Computing (WIHPQC)*, Online, New Mexico, United States, 2021-10-20 - 2021-10-20. (LA-UR-21-29917)

Pakin, S. D. Project Appraisal: Unifying Circuit-Model Quantum Computing and Quantum Annealing (20210397ER). . (LA-UR-21-31655)

Wilson, E., F. Mueller and S. D. Pakin. Mapping Constraint Problems onto Quantum Gate and Annealing Devices. Presented at *Second International Workshop on Quantum Computing Software*, St. Louis, Missouri, United States, 2021-11-15 - 2021-11-15. (LA-UR-21-30483)

Posters

Wilson, E. J., F. Mueller and S. D. Pakin. NchooseK: Constraint Based Quantum Computing. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22086)

Resolving the Energy Transfer from a Nuclear Energy Source to the Ground

Esteban Rougier
20210436ER

Project Description

The main objective of this theoretical and computational project is to obtain a better understanding of the energy transfer mechanisms between a nuclear weapon surface burst and the surrounding solid media. The expected result is to reach an uncertainty reduction for cratering and lofted volume (ground and nearby materials being lifted into the atmosphere) estimates, thereby improving confidence on how much material would be available for radioactive fallout to occur for a particular nuclear event. A correlated result is to improve the fidelity of simulated nuclear weapons effects on both above ground and underground structures and facilities. Regarding the impact on Department of Energy/National Nuclear Security Administration missions, it has been recognized that to be able to predict the effects of a nuclear weapon detonation in a local and regional context is critical to planning for and responding to a nuclear detonation. Recent computer advances and computational techniques now allow us to tackle these challenges that we were previously unable to address. This effort sets a cornerstone in our pathway to improve the fidelity of nuclear weapon application scenario estimates, which are critical for National Command Authority decision making processes.

Publications

Journal Articles

*Lei, Z., E. Rougier, E. E. Knight, M. Zang and A. Munjiza. Impact Fracture and Fragmentation of Glass via the 3D Combined Finite-Discrete Element Method. 2021. *Applied Sciences*. **11** (6): 2484. (LA-UR-21-21493 DOI: 10.3390/app11062484)

Rougier, E. and A. Hunter. Fracture Mechanics—Theory, Modeling and Applications. 2021. *Applied Sciences*. **11** (16): 7371. (LA-UR-21-27423 DOI: 10.3390/app11167371)

Reports

Till, A. T. Discretization Writeup for Grey Flux-Limited Radiation Diffusion. Unpublished report. (LA-UR-20-29323)

Presentation Slides

Knight, E. E., Z. Lei, B. J. Euser, S. H. S. Boyce, A. Munjiza and E. Rougier. HOSS OVERVIEW. . (LA-UR-21-29085)

Lei, Z., E. E. Knight, E. Rougier, B. J. Euser, S. H. S. Boyce and A. Munjiza. Enhanced Contact and Fracture Solutions for FDEM. Presented at *WCCM-ECCOMAS 2020*, Barcelona, Spain, 2021-01-11 - 2021-01-15. (LA-UR-20-30016)

Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. The Combined Finite-Discrete Element Method (FDEM): An Overview. . (LA-UR-21-29098)

Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. The Combined Finite-Discrete Element Method (FDEM): An Overview. . (LA-UR-21-29089)

Rougier, E., E. E. Knight, Z. Lei, B. J. Euser, S. H. S. Boyce and A. Munjiza. LANL HOSS Modeling Capabilities. . (LA-UR-21-29065)

Rougier, E., Z. Lei, B. J. Euser, A. Munjiza and E. E. Knight. Fluid-Solid Interaction via the Combined Finite-Discrete Element Method. . (LA-UR-21-24172)

Rougier, E., Z. Lei, B. J. Euser, E. E. Knight and A. Munjiza. Fluid-Structure Interaction Problems via the Combined Finite-Discrete Element Method. Presented at *14th World COngress on Computational Mechanics*, Paris, France, 2021-01-11 - 2021-01-11. (LA-UR-20-29727)

Mimetic Tensor-Train Algorithms for High-Dimensional Partial Differential Equations (PDEs) without the Curse of Dimensionality

Gianmarco Manzini
20210485ER

Project Description

This project will focus on two very specific goals: (i) developing numerical methods for solving high-dimensional partial differential equations (PDEs), and (ii) developing numerical methods for solving PDEs with a high number of degrees of freedom. This is a basic research project with immense potential impact; this project's results can potentially be a "game changer" in the compute treatment in a variety of fields and applications, including national engineering problems that require massive numerical simulations.

Publications

Journal Articles

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Submitted to *Numerical Linear Algebra with Applications*. (LA-UR-21-26100)

Conference Papers

Manzini, G., E. W. Skau, P. M. D. Truong and R. Vangara. Nonnegative tensor-train low-rank approximations of the Smoluchowski equation. Presented at *13th International Conference on "Large-Scale Scientific Computations"*. (Sozopol, Bulgaria, 2021-06-07 - 2021-06-11). (LA-UR-21-23325)

Reports

Alexandrov, B., G. Manzini, E. W. Skau and P. M. D. Truong. Composite numerical integration on the multidimensional hypercube using low-rank tensor-train cross representation. Unpublished report. (LA-UR-21-24664)

Manzini, G., B. Alexandrov, K. O. Rasmussen and P. M. D. Truong. White paper - Ultra-fast Tensor Solvers for Ultra-big PDEs. Unpublished report. (LA-UR-21-30691)

Presentation Slides

Alexandrov, B., G. Manzini, E. W. Skau, P. M. D. Truong and R. Vuchkov. Tensor Train Network and its Applications to Numerical Integration and Partial Differential Equations. Presented at *Optimization Seminar, University of California, Merced*, Merced, California, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-29268)

Manzini, G. A non-negative tensor-train based method for the Smoluchowski coagulation equation.. Presented at *13th International Conference on Large-Scale Scientific Computations*, Sozopol, Bulgaria, 2021-06-07 - 2021-06-11. (LA-UR-21-25537)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *16th U.S. National Congress on Computational Mechanics (USNCCM-16)*, Chicago, Illinois, United States, 2021-07-25 - 2021-07-29. (LA-UR-21-25539)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *SIAM Conference on Mathematical & Computational Issues in the Geosciences (GS21)*, Milano, Italy, 2021-06-21 - 2021-06-24. (LA-UR-21-25538)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *16th U.S. National Congress on Computational Mechanics (USNCCM-16) - LA-UR-21-25539*, Chicago, Illinois, United States, 2021-07-25 - 2021-07-29. (LA-UR-21-25671)

Manzini, G. The arbitrary-order virtual element method for linear elastodynamics models. Presented at *SIAM Conference on Mathematical & Computational Issues in the Geosciences (GS21)*, Milano, Italy, 2021-06-21 - 2021-06-24. (LA-UR-21-25672)

Accelerating Parallel Transport Sweeps with Fully Asynchronous Graph Traversal

David Dixon
20210835ER

Project Description

Radiation transport sweep algorithms take the largest fraction of time in important simulations conducted at Los Alamos National Laboratory (LANL) - roughly 50% of the total time. Even a modest improvement in efficiency would be an extraordinary contribution to laboratory scientists that run simulations. This work could broadly impact LANL high-performance computing (HPC) multiphysics efforts by: (1) greatly improving transport sweep parallel efficiency through a novel application of an asynchronous programming model; (2) decreasing turn-around time in expensive LANL multiphysics simulations opening the door to currently intractable problems; (3) providing future exascale computing efforts with insight into how conventional and novel parallel runtimes and performance-portability ecosystems might coexist in a multiphysics application; (4) exploring new approaches to transport sweeps on heterogeneous platforms by mixing task execution on different architectures; and (5) most importantly, being the first body of work to investigate how the use of billions of light-weight, asynchronous tasks can improve performance of parallel radiation transport sweeps and associated applications.

Monte Carlo Transport Simulations on a Billion-Core Approximate-Computing Platform

Alex Long
20210849ER

Project Description

Through this project we will explore a different type of computer that is faster and uses less power but it has some imprecise arithmetic. If we can adapt an important physics algorithm to work well on this new computer we have a chance to greatly improve the workflows of users in the National Nuclear Security Administration (NNSA).

Publications

Presentation Slides

Long, A. R. An Overview of the Implicit Monte Carlo Algorithm. . (LA-UR-21-23650)

Pakin, S. D. Computing Logarithms on S1 Hardware. . (LA-UR-22-21367)

Shape Matching of 3-Dimensional Computer-Aided Design (CAD) Models in Automatic Hexahedral Meshing Workflows

Rao Garimella
20210906ER

Project Description

Many national security applications, including performance assessments of nuclear and conventional weapons systems, involve complex multiphysics simulations. These simulations require the domain (or geometric model) to be tiled with simpler shapes called hexahedral elements to form a computational mesh Generating these meshes is at best a semi-automatic process guided by experienced analysts and can take up as much 50% of the design-analysis cycle time. Our research will apply machine learning techniques to match input geometries to models that the system already knows how to decompose and mesh. This project will serve as proof of principle that such shape matching is possible without huge training data sets. In the short term, we expect to be able to identify "dirty geometry" (unexpected hidden geometric modeling artifacts) that trip up engineers trying to mesh the models. The long term plan of using machine learning for hexahedral meshing holds the promise of capturing the intuition of experienced engineers by "learning" general strategies for meshing such models. This will eventually have far-ranging impacts in many Department of Energy (DOE) applications with national security implications, including weapons system performance, seismic monitoring for non-proliferation, nuclear energy production and others.

Publications

Conference Papers

Garimella, R. V., C. Garcia Cardona and N. Ray. AI for Automatic Hexahedral Meshing. Presented at *AI@DOE (https://www.orau.gov/AI-DOERoundtable)*. (Virtual, New Mexico, United States, 2021-12-01 - 2021-12-01). (LA-UR-21-31688)

Reports

Payne, E. R., N. Ray, R. V. Garimella and C. Garcia Cardona. Shape Matching for Hexahedral Mesh Generation. Unpublished report. (LA-UR-21-28999)

Effects of Cosmic Ray Neutrons on Modern High Performance Computing (HPC) Components

Nathan Debardeleben
20180017ER

Project Description

Advanced supercomputer systems are using technologies and components of amazing scale and complexity. As we push into these extreme regions, we also greatly push the envelope in the reliability of the systems both in terms of productive use of the machine (utilization, throughput, uptime, etc.) but also in the integrity (correctness) of the calculations done on these systems. It is imperative that we fully understand the causes of interruptions on these extreme-scale systems so that we can better understand how to build and operate them not only for the next generation systems but also the computing industry. Today's extreme-scale supercomputers become tomorrow's corporate supercomputers for technical and economic innovation. To accomplish this, we will use historical data from LANL supercomputers to attribute causes to effects, particularly environmental effects, which are believed to be the primary cause for errors on these systems. Based on preliminary work by the team, we will deploy neutron detectors, correlate the rate with system events, model, and simulate the expected neutron impacts on the supercomputer using advanced software simulation tools. We will also study the effects of solar events (coronal mass ejections) and evaluate the efficacy of shielding the supercomputer from a variety of error sources.

Technical Outcomes

Thermal neutrons are an important aspect to be studied alongside fast neutrons in evaluating terrestrial computer system reliability. Coronal mass ejections can be observed through careful analysis of supercomputer error rates terrestrially and correlated with data from supercomputers across the country. This project developed a method of modeling datacenters and supercomputers and used the model to evaluate errors seen on these systems under testing. The team enhanced the thermal neutron detection technique and deployed it in the datacenter.

Publications

Journal Articles

Bowen, C. M., N. A. Debardeleben, S. P. Blanchard and C. M. Anderson-Cook. Do Solar Proton Events Reduce the Number of Faults in Supercomputers?: A Comparative Analysis of Faults during and without Solar Proton Events. Submitted to *IEEE International Reliability Physics Symposium*. (LA-UR-19-31047)

Oliveira, D., S. P. Blanchard, N. A. Debardeleben, F. F. dos Santos, G. Piscoya Dávila, P. Navaux, A. Favalli, O. M. Schappert, S. A. Wender, C. Cazzaniga, C. Frost and P. Rech. Thermal Neutrons: a Possible Threat for Supercomputer Reliability. Submitted to *Journal of Supercomputing*. (LA-UR-20-23114)

Conference Papers

Blanchard, S. P., N. A. Debardeleben, P. Rech and D. Oliveira. Thermal Neutrons: A New Threat for Supercomputers and Safety Critical Applications. Presented at *SC'19*. (Denver, Colorado, United States, 2019-11-17 - 2019-11-17). (LA-UR-19-23232)

Oliveira, D., S. P. Blanchard, N. A. Debardeleben, F. F. dos Santos, G. P. D\xc3\xa1vila, P. Navaux, S. A. Wender, C. Cazzaniga, C. Frost, R. Baumann and P. Rech. An Overview of the Risk Posed by Thermal Neutrons to the Reliability of Computing Devices. Presented at *50th IEEE/IFIP Int. Conference on Dependable Systems and Networks*. (Valencia, Spain, 2020-06-29 - 2020-07-02). (LA-UR-20-23268)

Reports

Wender, S. A., A. J. Couture and T. D. Fairbanks. Report on the Tin-II Thermal Neutron Detector. Unpublished report. (LA-UR-19-30822)

Presentation Slides

Bowen, C. M. Telling a Visual Story within Big Data: Case Studies on Interactive Visualizations for Supercomputer Data. Presented at *Rising Stars in Computational and Data Sciences*, Austin, Texas, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-22930)

Bowen, C. M. Telling a visual story within big data: case studies on interactive visualizations for supercomputer data. Presented at *21st Meeting of New Researchers in Statistics and Probability*, Fort Collins, Colorado, United States, 2019-07-24 - 2019-07-24. (LA-UR-19-26857)

Bowen, C. M., N. A. Debardeleben, S. P. Blanchard and C. M. Anderson-Cook. Do Solar Proton Events Reduce the Number of Faults in Supercomputers?: A Comparative Analysis of Faults during and without Solar Proton Events. Presented at *2019 Institute of Electrical and Electronics Engineers International Reliability Physics Symposium*, Monterey, California, United States, 2019-03-31 - 2019-03-31. (LA-UR-19-22250)

R. Mullin, E. R., S. F. Nowicki, N. A. Debardeleben, S. P. Blanchard, S. A. Wender and E. A. Baseman. Pre-deployment Characterization of Large Fast Neutron Detectors for High Performance Computing Fault Characterization. Presented at *2018 Symposium on Radiation Measurements and Applications (SORMA XVII)*, Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-14. (LA-UR-18-21582)

Nowicki, S. F., L. Ferres, E. R. R. Mullin, S. P. Blanchard, N. A. Debardeleben, S. A. Wender and G. E. McMath. Neutron Environment at High-Altitude High-Performance Computing Facilities. Presented at *NSREC*, Santa Fe, New Mexico, United States, 2020-10-30 - 2020-10-30. (LA-UR-20-28797)

Oliveira, D., S. P. Blanchard, N. A. Debardeleben, F. dos Santos, G. Piscoya, P. Navaux, S. A. Wender, C. Cazzaniga, C. Frost, R. Baumann and P. Rech. Thermal Neutrons: a Possible Threat for Supercomputers and Safety Critical Applications. Presented at *SELSE 2020*, Stanford, California, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-23267)

Ortega, S. P., N. A. Debardeleben and C. M. Bowen. Differential Privacy for Supercomputer Sensor Data. Presented at *USRC and HPC Symposia*, Los Alamos, New Mexico, United States, 2019-07-31 - 2019-08-01. (LA-UR-19-27434)

Ortega, S. P., N. A. Debardeleben and C. M. Bowen. Differential Privacy for Supercomputer Sensor Data. . (LA-UR-19-27097)

Schappert, O. M., S. P. Blanchard, N. A. Debardeleben, R. E. Lakis and A. Favalli. MCNP Simulations of Neutron Fluxes Through Trinity Supercomputer Nodes. . (LA-UR-19-27755)

Posters

Bowen, C. M. Telling a Visual Story within Big Data: Case Studies on Interactive Visualizations for Supercomputer Data. Presented at *Spring Research Conference*, Blacksburg, Virginia, United States, 2019-05-22 - 2019-05-22. (LA-UR-19-24529)

Debardeleben, N. A. Data Analytics for Neutron Detection. Presented at *Ultrascale Systems Research Center Research Symposium*, Los Alamos, New Mexico, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-27103)

Massively-Parallel Acceleration of the Dynamics of Complex Systems: a Data-Driven Approach

Danny Perez
20190034ER

Project Description

Current atomistic modeling techniques are limited to extremely short timescales (on the order of microseconds or less), no matter the size of the computer that is used to carry out the simulations. This severely limits their ability to directly interpret experiments or to predict how materials will perform in real life. The key to addressing this problem is to find more efficient ways to exploit the computing power available via the Department of Energy's very large computers. We will develop and implement powerful massively-parallel algorithms deployed on thousands of processors in order to dramatically extend the range of systems that can be simulated over very long times. We will demonstrate the approach on a range of problems of interest to DOE, including the motion of dislocations in materials (materials failure in extreme conditions), the evolution of complex defects in nuclear materials (nuclear safety) and the evolution of bio-molecules (bio-security). In all of these cases, the lack of access to long-times has so far made computational materials design and drug design extremely challenging. Our goal is to use powerful algorithms and very-large-scale computing to directly tackle this challenge.

Technical Outcomes

The team developed a suite of powerful analysis algorithms that can intake simulation data in real-time as new simulation data is generated. These algorithms are able to analyze the dynamics on-the-fly, which allows for the detection and characterization of so-called "metastable" states. This detection and characterization has been exploited to develop powerful parallel algorithms that can greatly extend the simulation timescales of complex systems where human intuition fails at identifying and characterizing the dynamics.

Publications

Journal Articles

Lin, Y. T., Y. Tian, M. Anghel and D. Livescu. Data-driven learning for the Mori--Zwanzig formalism: a generalization of the Koopman learning framework. Submitted to *SIAM Journal on Applied Dynamical Systems*. (LA-UR-21-20187)

Perez, D., A. Agarwal, A. F. Voter and S. Gnanakaran. Arbitrary accurate representation of atomistic dynamics via semi-Markov jump processes. Submitted to *TBD*. (LA-UR-19-29252)

Perez, D., M. Boleininger, M. Gallauer, S. Dudarev, T. Swinburne and D. Mason. Statistical mechanics of kinks on a gliding screw dislocation. Submitted to *TBD*. (LA-UR-20-23814)

Tian, Y., Y. T. Lin, M. Anghel and D. Livescu. Data Driven Learning of Mori-Zwanzig Operators for Isotropic Turbulence. Submitted to *Physics of Fluids*. (LA-UR-21-28283)

Presentation Slides

Mathew, N., E. Martinez Saez and D. Perez. Accelerated Molecular Dynamics Simulations of Dislocation-Obstacle Interactions in Tungsten: Enabling Micro-Second Simulations. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22073)

Mathew, N., E. Martinez and D. Perez. Investigating Dislocation-Obstacle Interactions in Tungsten using a novel Parallel Replica Dynamics Method. Presented at *APS March Meeting 2021*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22342)

Perez, D. Complex High-Dimensional Energy Landscapes. Presented at *Reunion workshop of the Complex High-Dimensional Energy Landscapes program.*, Lake Arrowhead, California, United States, 2019-06-10 - 2019-06-10. (LA-UR-19-25405)

Objective Flow Topology

Roxana Bujack
20190143ER

Project Description

High Explosives safety and surety and nuclear energy research rely heavily on computational simulations. DOE's supercomputers, expert scientists, and advanced hydrodynamics codes produce ever increasing datasets. This creates new challenges. First, while computational resources are increasing in modern high performance computing (HPC) architectures, the capacity for loading and storing data is not keeping pace- in effect, more data is produced than can be stored. The second problem is that scientists cannot view and comprehend ever larger amounts of flow data during visual analysis because human vision has finite resolution. Our proposed method will solve both problems by providing the means to better analyze big flow data by reducing it to its most essential structure. Firstly, it compresses the data, which helps overcome the Input/Output (I/O) bottleneck and allows the analysis of huge simulation data on a desktop machine with minimal loss of relevant information. Secondly, it produces a decluttered visualization of the fundamental behavior of the flow with minimal occlusion from less important regions.

Technical Outcomes

The team has successfully developed a method to generalize vector field topology to be objective using the contraction and expansion patterns of pathlines in analogy to the asymptotic streamline patterns around classical critical points. They further collected conditions for time-dependent flow topology to be physically meaningful and evaluated all existing approaches based on these criteria. Finally, the team published an open source vector field topology algorithm in the Visualization Toolkit (VTK).

Publications

Journal Articles

Bujack, R. B., E. Bresciani, J. Waters and W. Schroeder. Topological Segmentation of 2D Vector Fields. Submitted to *Computers And Graphics*. (LA-UR-21-21785)

*Bujack, R. B., K. C. Tsai, S. K. Morley and E. Brescani. Open source vector field topology. 2021. *SoftwareX*. **15**: 100787. (LA-UR-20-29277 DOI: 10.1016/j.softx.2021.100787)

*Bujack, R. and A. Middel. State of the art in flow visualization in the environmental sciences. 2020. *Environmental Earth Sciences*. **79** (2): 65. (LA-UR-19-31637 DOI: 10.1007/s12665-019-8800-4)

Conference Papers

Bujack, R. B. Visualization of Distinguished Trajectories as a Generalization of Critical Points to Time-dependent Flow. Presented at *IEEE VIS*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-20-23159)

Bujack, R. B. Comparison of Different Methods to Extract Vector Field Topology on Finite Domains. Presented at *IEEE VIS*. (New Orleans, Louisiana, United States, 2021-10-24 - 2021-10-24). (LA-UR-21-20582)

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. Time-Dependent Flow Topology: Past, Present, and Future. Presented at *EuroVis*. (Lingkoeping, Sweden, 2020-06-03 - 2020-06-03). (LA-UR-19-30267)

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. State of the Art in Time-Dependent Flow Topology: Interpreting Physical Meaningfulness Through Mathematical Properties. Presented at *EuroVis*. (Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25). (LA-UR-20-23019)

Bujack, R. B., S. Dutta, D. Z. Zhang and T. Gunther. Objective Finite-Time Flow Topology from Flowmap Expansion and Contraction. Presented at *TopoInVis*. (Nyk\xc3\xb6ping, Sweden, 2019-06-17 - 2019-06-19). (LA-UR-19-23386)

Bujack, R. B., S. Dutta, I. B. Rojo, D. Z. Zhang and T. G \xc3\xbcnther. Objective Finite-Time Saddles and their Connection to FTLE. Presented at *EuroVis 2019*. (Porto, Portugal, 2019-06-03 - 2019-06-07). (LA-UR-19-21831)

Bujack, R. B., S. Sane, C. Garth and H. Childs. Survey of Seed Placement and Streamline Selection Techniques. Presented at *EuroVis*. (Linkoeping, Sweden, 2019-06-03 - 2019-06-03). (LA-UR-19-30263)

Dutta, S., R. X. Brady, M. E. Maltrud, P. J. J. Wolfram and R. B. Bujack. Leveraging Lagrangian Analysis for Discriminating Nutrient Origins. Presented at *Visualization*

in Environmental Sciences. (Porto, Portugal, 2019-06-03 - 2019-06-03). (LA-UR-19-22455)

Yan, L., B. Wang and R. B. Bujack. Finite-time Saddles from Particle Origin and Destination. Presented at *Eurovis 2020*. (Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25). (LA-UR-19-26219)

Books/Chapters

Hotz, I., R. B. Bujack, C. Garth and B. Wang. Mathematical Foundations in Visualization. (LA-UR-19-29121)

Reports

Bujack, R. B. The Definition of a Separatrix. Unpublished report. (LA-UR-21-22238)

Bujack, R. B. Visualization Showcases. Unpublished report. (LA-UR-21-29064)

Bujack, R. B., N. W. Birge, V. Geppert-Kleinrath, P. L. Volegov and D. H. Rogers. Topological Analysis for Fusion Ignition. Unpublished report. (LA-UR-21-29431)

Presentation Slides

Bujack, R. B. State of the Art in Time-Dependent Flow Topology: Interpreting Physical Meaningfulness Through Mathematical Properties. Presented at *EuroVis*, Norrk \xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25. (LA-UR-20-23457)

Bujack, R. B. Vector Field Topology. . (LA-UR-21-23756)

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. State of the Art in Time-Dependent Flow Topology: Interpreting Physical Meaningfulness Through Mathematical Properties. Presented at *EuroVis*, Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25. (LA-UR-20-23456)

Other

Bujack, R. B. Vector Field Topology. Audio/Visual. (LA-UR-21-23904)

Towards Memristor Supremacy with Novel Machine Learning Algorithms

Francesco Caravelli
20190195ER

Project Description

Memristors are the nanoscale equivalent of brain synapses: these are passive components able to learn, and their prospective application is in reproducing the capabilities of the brain. This project is a first step towards the integration of (hard) computational tasks in dense nanoscale analog circuits. The success of this project will show that the use of memristors without a complementary metal oxide semiconductor (CMOS), the base for current computational architectures, can still be used for storage and low-energy computation. The addition of CMOS hardware will then be used for hybrid brain-like and digital-like computers. This project is aligned with the goal of "Beyond Moore's Law" computation, one the Department of Energy missions. While some brain-like chips are currently available, their architecture is simple; the purpose of this project is to go beyond standard architectures.

Technical Outcomes

During this project we have developed an experimentally rooted approach to memristor chips, and a new algorithm and machine learning algorithms based on memristor behavior. The project designed and operated memristor based circuits (memristor synapses) for optimization purposes. As such, we have initiated a new area of research in machine learning, inspired by memristive circuits, for neuromorphic dynamical systems, which can be applied to general machine learning algorithms and not based on a Turing paradigm.

Publications

Journal Articles

C. F. *. C. F. *. V. P. Bartolucci, S. *. and F. Caravelli. "Spectrally gapped" random walks on networks: a Mean First Passage Time formula. 2021. *SciPost Physics*. **11** (5): 088. (LA-UR-21-25315 DOI: 10.21468/SciPostPhys.11.5.088)

Ben-Naim, E. and P. L. Krapivsky. Monotonicity in averaging processes. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-21-28699)

*Caravelli, F. Asymptotic Behavior of Memristive Circuits. 2019. *Entropy*. **21** (8): 789. (LA-UR-18-24748 DOI: 10.3390/e21080789)

Caravelli, F. Inversion-free Leontief inverse: statistical regularities in input-output analysis from partial information. Submitted to *Revista Mexicana de Fisica*. (LA-UR-20-26892)

Caravelli, F., C. Nisoli and G. Chern. Phase-change spin ice memory resistor. Submitted to *Physical Review Letters*. (LA-UR-19-27438)

Caravelli, F., F. C. Sheldon and F. L. Traversa. Tunneling through barrier by passive dynamical system. Submitted to *Physical Review Letters*. (LA-UR-20-28084)

Caravelli, F., F. C. Sheldon and F. L. Traversa. Global minimization via classical tunneling assisted by collective force field formation. 2021. *Science Advances*. **7** (52): eabh1542. (LA-UR-21-20810 DOI: 10.1126/sciadv.abh1542)

Caravelli, F., S. Bartolucci, F. Caccioli and P. Vivo. Universal Rankings in complex input-output organizations. Submitted to *Nature*. (LA-UR-20-27058)

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

*Caravelli, F. and J. P. Carbajal. Memristors for the Curious Outsiders. 2018. *Technologies*. **6** (4): 118. (LA-UR-18-27766 DOI: 10.3390/technologies6040118)

Pang, Y., C. J. Coffrin, A. Lokhov and M. D. Vuffray. The potential of quantum annealing for rapid solution structure identification. 2020. *Constraints*. (LA-UR-20-22733 DOI: 10.1007/s10601-020-09315-0)

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

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

*Zegarac, A. and F. Caravelli. Memristive networks: From graph theory to statistical physics. 2019. *EPL (Europhysics Letters)*. **125** (1): 10001. (LA-UR-18-31372 DOI: 10.1209/0295-5075/125/10001)

Conference Papers

Coffrin, C. J., H. Nagarajan and R. W. Bent. Evaluating Ising Processing Units with Integer Programming. Presented at *Sixteenth International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Thessaloniki, Greece, 2019-06-04 - 2019-06-07). (LA-UR-19-22000)

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

Jayakumar, A., A. Lokhov, S. Misra and M. D. Vuffray. Learning of Discrete Graphical Models with Neural Networks. Presented at *NeurIPS*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-24927)

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

Pang, Y., C. J. Coffrin, A. Lokhov and M. D. Vuffray. The Potential of Quantum Annealing for Rapid Solution Structure Identification. Presented at *17th International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Vienna, Austria, 2020-05-26 - 2020-05-29). (LA-UR-19-31884)

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

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *NeurIPS 2020*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-25018)

Books/Chapters

Sheldon, F. C., C. J. Coffrin and F. Caravelli. Fully analog memristive circuits for optimization tasks: a comparison. (LA-UR-20-26683)

Reports

Caravelli, F. Towards memristor supremacy with novel machine learning algorithms. Unpublished report. (LA-UR-21-29523)

Presentation Slides

Caravelli, F. Memristive Networks. Presented at *Talk @ICTP Trieste*, Trieste, Italy, 2019-09-23 - 2019-09-23. (LA-UR-19-29539)

Caravelli, F. Computing with memristive devices and networks. . (LA-UR-20-29385)

Caravelli, F. Memristor Networks. Presented at *SIFS - Societa Italiana di Fisica Statistica*, Parma, Italy, 2021-06-23 - 2021-06-25. (LA-UR-21-25862)

Coffrin, C. J. Beyond Moore's Law: Exploring the Future of Computation. . (LA-UR-19-21268)

Coffrin, C. J. Novel Computing Platforms: Potential and Challenges for Discrete Optimization. . (LA-UR-19-21267)

Coffrin, C. J. Challenges with Chains: Testing the Limits of a D-Wave Quantum Annealer for Discrete Optimization. . (LA-UR-19-21739)

Coffrin, C. J. Harnessing Analog Noise: A Hybrid Algorithm for Binary Quadratic Optimization with Uncertainty. . (LA-UR-19-24684)

Coffrin, C. J. The Potential of Quantum Annealing for Rapid Solution Structure Identification. . (LA-UR-20-21046)

Lokhov, A. Uncovering the behavior of quantum annealers with statistical learning. Presented at *APS march meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-22165)

Lokhov, A. Uncovering the behavior of quantum annealers with statistical learning. Presented at *At the crossroads of physics and machine learning*, Santa Barbara, California, United States, 2019-02-11 - 2019-02-11. (LA-UR-19-22163)

Lokhov, A. Learning Discrete Graphical Models with Neural Networks. Presented at *Youth in High-dimensions: Machine Learning, High-dimensional Statistics and Inference for the New Generation*, Online, New Mexico, United States, 2020-06-29 - 2020-06-29. (LA-UR-20-24925)

Lokhov, A. Learning of Discrete Graphical Models: Ising, Potts, and beyond. Presented at *Statistical mechanics methods for networks*, Online, New Mexico, United States, 2020-09-17 - 2020-09-17. (LA-UR-20-27372)

Sheldon, F. C., A. Kolchinsky and F. Caravelli. The Computational Capacity of Mem-LRC Networks. Presented at *NICE*, NICE, Germany, 2021-03-09 - 2021-03-09. (LA-UR-21-22337)

Vuffray, M. D., C. J. Coffrin, Y. Kharkov and A. Lokhov. Programmable Quantum Annealers as Noisy Gibbs Samplers. Presented at *Adiabatic Quantum Comouting Conference (AQC) 2021*, Tokyo, Japan, 2021-06-22 - 2021-06-25. (LA-UR-21-25991)

Vuffray, M. D., S. Misra and A. Lokhov. Learning Discrete Graphical Models Exact & Neural Assisted Methods. Presented at *IMA: Theory and Algorithms in Graph-based Learning workshop*, Mineapolis, Minnesota, United States, 2020-09-14 - 2020-09-18. (LA-UR-20-27337)

Posters

Lokhov, A. Optimal deployment of resources for maximizing impact in spreading processes. Presented at *APS march meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-22164)

Other

Coffrin, C. J. The Potential of Quantum Annealing for Rapid Solution Structure Identification (video). Audio/Visual. (LA-UR-20-23778)

Stable, Conservative, High-Order Numerical Methods for Direct Numerical Simulations (DNS) in Complex Geometries

Peter Brady
20190227ER

Project Description

Numerical simulations play a key role in stockpile stewardship. The large scale industrial simulations that are required for understanding the complex regimes arising from stockpile stewardship considerations employ a variety simplified physical models. The development and assessment of these models can be greatly enhanced by reliable databases produced by more focused, high-fidelity simulations. This project will extend the capabilities of high-fidelity, exa-scale simulations to the complex configurations that are typically encountered in engineering applications.

Technical Outcomes

This project successfully demonstrated the use of of a novel optimization procedure to produce high-order finite-difference approximations that yield stable discretizations for a range of partial differential equations and boundary condition combinations. These combinations are representative of what will be encountered in simulations compressible turbulent flow in regimes of interest to Los Alamos. This novel strategy was the subject of journal articles, numerous conference presentations, and implemented in the new open source solver, SHOCCS software.

Publications

Journal Articles

*Brady, P. T. and D. Livescu. Foundations for high-order, conservative cut-cell methods: Stable discretizations on degenerate meshes. 2021. *Journal of Computational Physics*. **426**: 109794. (LA-UR-20-22279 DOI: 10.1016/j.jcp.2020.109794)

Sharan, N., P. T. Brady and D. Livescu. Time-stable strong boundary conditions in finite-difference schemes for hyperbolic systems. Submitted to *Journal of Computational Physics*. (LA-UR-20-24938)

Conference Papers

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-Cell Methods. Presented at *AIAA Scitech*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-29984)

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-Cell Methods. Presented at *AIAA SciTech Forum*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-31402)

Sharan, N., M. Natarajan, P. T. Brady and D. Livescu. A deep learning framework for derivation of time-stable difference schemes. Presented at *2021 AIAA Aviation Forum*. (Virtual, New Mexico, United States, 2021-08-02 - 2021-08-06). (LA-UR-21-27459)

Sharan, N., P. T. Brady and D. Livescu. Stable and conservative boundary treatment for difference methods, with application to cut-cell discretizations. Presented at *2020 AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-32707)

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. Numerical Study of the Properties of a Ghost-Cell Method. Presented at *American Institute of Aeronautics and Astronautics*. (Orlando, Florida, United States, 2020-01-07 - 2020-01-11). (LA-UR-19-28614)

Reports

Brady, P. T. and D. Livescu. High-Order, Stable, and Conservative Boundary Schemes for Central and Compact Finite Differences. Unpublished report. (LA-UR-19-20056)

Presentation Slides

Brady, P. T. and D. Livescu. A Foundation for High-Order Cut-Cell Methods: Stable Derivatives on Degenerate Meshes. Presented at *APS DFD*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-30896)

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-cell Methods. Presented at *AIAA Scitech*, San Diego, California, United States, 2019-01-07 - 2019-01-07. (LA-UR-19-20057)

Brady, P. T. and D. Livescu. High-Order Cut-Cell Methods in Multiple Dimensions. Presented at *72nd APS DFD*

meeting, Seattle, Washington, United States, 2019-11-23 - 2019-11-23. (LA-UR-19-31797)

Kim, K. H. Composition and Dynamical Processes of Ions in Giant Magnetospheres: The Importance of In Situ Measurements for Advancing the Current Knowledge. . (LA-UR-20-28874)

Sharan, N., P. T. Brady and D. Livescu. High-order energy-stable boundary treatment for finite-difference cut-cell method. Presented at *72nd Annual Meeting of the APS Division of Fluid Dynamics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31665)

Sharan, N., P. T. Brady and D. Livescu. Stable and conservative boundary treatment for difference methods, with application to cut-cell discretizations. Presented at *2020 AIAA SciTech Forum*, Orlando, Florida, United States, 2020-01-06 - 2020-01-06. (LA-UR-20-20086)

Sharan, N., P. T. Brady and D. Livescu. Dimensionally-split provably stable cut-cell approach for flow calculations. Presented at *APS Division of Fluid Dynamics Meeting 2020*, Online, New Mexico, United States, 2020-11-22 - 2020-11-24. (LA-UR-20-29646)

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. High-Order Ghost-Cell Method for Non-Conforming Boundaries. Presented at *American Physical Society Division of Fluid Dynamics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31645)

Posters

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. High-Order Ghost-Point Method for Non-Conforming Boundaries. Presented at *Los Alamos Post-doc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28565)

Statistical Learning in Cyberphysical Systems

Nathan Lemons
20190351ER

Project Description

The overarching goal of this project is to develop novel data-driven algorithms for statisical learning of an effective high-fidelity representation of cyberphysical systems. This will allow applications such as real-time detection and classification of anomalies, state estimation for damage-recovery operations, and optimal expansion of the system. We expect our work to be highly relevant to those tasked with operating and protecting large networked cyberphysical systems, such as electric grids. This research is directly relevant to the program office "Cybersecurity for Energy Delivery Systems" within the Office of Electricity in the Department of Energy. It is expected that members of the Intelligence Community will also be interested in this work. We also expect to contribute to the state of the art in machine learning and statistical learning through publications and presentations at top conferences.

Technical Outcomes

The team successfully developed algorithms for the learning of purely discrete systems; the learning of purely continuous systems; the learning of mixed (discrete and continuous systems); the learning of systems with partial information. These algorithms were tested on synthetic and real data including power grid data. Our work was publicized in several high quality publications and presented at the top machine learning, mathematics, power systems, and control conferences.

Publications

Journal Articles

*L. N. *. P. C. BALOGH, J. *. and N. A. T. H. A. N. LEMONS. Maximum Size Intersecting Families of Bounded Minimum Positive Co-degree. 2021. *SIAM Journal on Discrete Mathematics*. **35** (3): 1525-1535. (LA-UR-20-23462 DOI: 10.1137/20M1336989)

Chertkov, M., V. Y. Chernyak and Y. Maximov. Gauges, Loops, and Polynomials for Partition Functions of Graphical Models. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-20-30432)

*L. N. *. S. N. *. Z. O. Gyori, E. *. and N. Lemons. The structure of hypergraphs without long Berge cycles. 2021. *Journal of Combinatorial Theory, Series B*. **148**: 239-250. (LA-UR-18-31512 DOI: 10.1016/j.jctb.2020.04.007)

Keszegh, B., N. W. Lemons, R. R. Martin, D. P\xc3\xa1lv\xc3\xb6lgyi and B. Patk\xc3\xb3s. Induced and non-induced poset saturation problems. Submitted to *SIAM Journal on Discrete Mathematics*. (LA-UR-20-22232)

Lemons, D. S., N. W. Lemons and W. Peter. Benford's Law and the Unbiased Sparse Partitioning of a Conserved Quantity. Submitted to *Physical Review E*. (LA-UR-20-23463)

Lemons, D., N. W. Lemons and W. Peter. First Digit Oscillations. Submitted to *MDPI Journal Stats*. (LA-UR-21-24136)

*Likhosherstov, V., Y. Maximov and M. Chertkov. Tractable minor-free generalization of planar zero-field Ising models. 2020. *Journal of Statistical Mechanics: Theory and Experiment*. **2020** (12): 124007. (LA-UR-19-30102 DOI: 10.1088/1742-5468/abcaf1)

Oles, V., N. W. Lemons and A. Panchenko. EFFICIENT ESTIMATION OF A GROMOV–HAUSDORFF DISTANCE BETWEEN UNWEIGHTED GRAPHS. Submitted to *IEEE Transactions on Pattern Analysis and Machine Intelligence*. (LA-UR-19-28284)

Conference Papers

Deka, D., U. Hashmi, L. Pereira, A. Busic and S. N. Backhaus. Co-optimizing Energy Storage for Prosumers using Convex Relaxations. Presented at *ISAP Conference 2019*. (New Delhi, India, 2019-12-10 - 2019-12-14). (LA-UR-19-29297)

Deka, D. and S. Misra. Learning for DC-OPF: Classifying active sets using neural nets. Presented at *Powertech 2019*. (milan, Italy, 2019-06-23 - 2019-06-27). (LA-UR-19-24726)

Hannon, C. M., D. Deka, D. Jin, M. D. Vuffray and A. Lokhov. Real-time Anomaly Detection and Classification in Streaming PMU Data. Presented at *XXI Power Systems Computation Conference*. (Porto, Portugal, 2020-06-29 - 2020-07-03). (LA-UR-19-31329)

Misra, S., M. D. Vuffray and A. Lokhov. Information Theoretic Optimal Learning of Gaussian Graphical Models.

Presented at *Conference on Learning Theory*. (Online, New Mexico, United States, 2020-07-09 - 2020-07-09). (LA-UR-20-24929)

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

Vuffray, M. D., S. Misra and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *NeurIPS 2020*. (Online, New Mexico, United States, 2020-12-05 - 2020-12-05). (LA-UR-20-25018)

Reports

Belyy, A., A. Sholokhov, M. R. Amini and Y. Maximov. MEMOIR: Multi-class Extreme Classification with Inexact Margin. Unpublished report. (LA-UR-19-21219)

Burashnikova, A., Y. Maximov and M. R. Amini. Sequential Learning over Implicit Feedback for Robust Large-Scale Recommender Systems. Unpublished report. (LA-UR-19-21349)

Krechetov, M., Y. Maximov, J. Marecek and M. Takac. Entropy-Penalized Semidefinite Programming. Unpublished report. (LA-UR-18-24430)

Likhosherstov, V., Y. Maximov and M. Chertkov. Inference and Sampling of K33-free Ising Models. Unpublished report. (LA-UR-19-26932)

Likhosherstov, V., Y. Maximov and M. Chertkov. A New Family of Tractable Ising Models. Unpublished report. (LA-UR-19-24712)

Maximov, Y., A. Burashnikova, N. Dante, M. Clausel, M. R. Amini and R. Stoica. Recommender systems : when memory matters. Unpublished report. (LA-UR-21-22659)

Presentation Slides

Deka, D., H. Doddi and A. Lokhov. Sample Optimal topology learning of linear dynamical systems. . (LA-UR-20-25926)

Hannon, C. M., D. Deka, M. D. Vuffray and A. Lokhov. Real-time Modeling and Anomaly Detection in Cyber-physical Systems. . (LA-UR-20-22487)

Lemons, N. W. Statistical Learning in Cyberphysical Systems. . (LA-UR-21-20316)

Lemons, N. W. Bounding Positive Co-Degree: New Tur\xc3\xa1n Problems for Hypergraphs. Presented at *SIAM Conference on Discrete Mathematics*, Online, Washington, United States, 2021-07-20 - 2021-07-20. (LA-UR-21-26951)

Lokhov, A. Learning Discrete Graphical Models with Neural Networks. Presented at *Youth in High-dimensions: Machine Learning, High-dimensional Statistics and Inference for the New Generation*, Online, New Mexico, United States, 2020-06-29 - 2020-06-29. (LA-UR-20-24925)

Lokhov, A. Learning of Discrete Graphical Models: Ising, Potts, and beyond. Presented at *Statistical mechanics methods for networks*, Online, New Mexico, United States, 2020-09-17 - 2020-09-17. (LA-UR-20-27372)

Posters

Hannon, C., D. Deka and A. Lokhov. Realtime Modeling and Anomaly Detection in Cyber-Physical Systems. Presented at *NeurIPS*, Los Alamos, New Mexico, United States, 2019-12-08 - 2019-12-14. (LA-UR-19-32246)

Impact of Mobility on Coronavirus (Covid-19) Spread

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20210709ER

Project Description

Human mobility is an important factor influencing the spread of epidemics, yet it is an open problem to determine how much mobility can be allowed while controlling an outbreak. The goal of the project is to develop empirically validated epidemic models that functionally relate human mobility to disease spread, thereby enabling the quantification of mobility control measures on disease spread. Existing epidemic models with mobility are either agent-based models or based on spatially coupled differential equations. Our approach differs. We seek to model the net effect of mobility on the response (incidence, death) using machine learning (nonparametric statistics) methods. Our stretch goal will be to develop a framework in which the impact of mobility for excess death can be tied back to the impact of mobility on coronavirus incidence time series. The innovations of this project are new epidemic models that incorporate explicitly the net impact of mobility to make predictions about the future course of an epidemic outbreak, and the use of machine learning and nonparametric statistics to estimate the functional relationship between mobility and outcome. Characterizing how mobility affects disease spread has clear benefits for decision makers that need to devise public health and economic policies.

Technical Outcomes

Human mobility that mixes infected and susceptible individuals is an important contributing factor in the spread of communicable diseases. As expected, we found that a decrease in mobility in prior weeks were statistically related to a decrease in excess deaths. Increased variability in mobility also increased excess deaths, indicating that the behavior of a minority of the population can impact the dynamic of an outbreak.

Publications

Journal Articles

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

*Cuellar-Hengartner, L., I. Torres, E. Romero-Severson, R. Mahesh, N. R. Ortega, S. A. Pungitore, R. Ke and N. W. Hengartner. Excess deaths reveal unequal impact of COVID-19 in Ecuador. 2021. *BMJ Global Health*. **6** (9): e006446.. (LA-UR-21-25221 DOI: 10.1136/bmjgh-2021-006446)

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

Presentation Slides

Cuellar-Hengartner, L., I. Torres, E. Romero-Severson, R. Mahesh, N. R. Ortega, S. A. Pungitore, N. W. Hengartner and R. Ke. Excess Deaths Reveal the enormous Impact of COVID-19 on Mortality and the role of the non-pharmaceutical Interventions in preventing deaths in Ecuador. Presented at *28th International Dynamics & Evolution of Human Viruses*, Virtual Meeting, California, United States, 2021-05-05 - 2021-05-07. (LA-UR-21-24230)

Hengartner, N. W. Estimating the epidemic growth rate and the reproductive number R0 of SARS-CoV-2. Presented at *American Physical Society annual confernece*, Virtual, New Mexico, United States, 2021-03-14 - 2021-03-19. (LA-UR-21-22646)

Hengartner, N. W. and C. Hengartner. The Science of COVID spread and prevention. . (LA-UR-21-23995)

Limited Information Tomography

Marc Klasky
20210723ER

Project Description

Dynamic radiography and computed tomography (CT) are among the flagship diagnostic and scientific capabilities at Los Alamos National Laboratory (LANL). CT reconstructs a 3-Dimensional (3D) volume from a set of its 2-Dimensional (2D) radiographic projections, typically requiring numerous projections (100s or 1000s) at angles evenly spaced between 0 and 180 degrees to accurately reconstruct a 3D volume. For applications such as Emergency Response or dynamic radiography only a limited set of views are possible. In numerous surveillance, production, or scientific activities the cost in time and dose to the part can be prohibitive. Developing the scientific and computational tools to provide high fidelity, rapid, 3D tomographic reconstructions from a limited number of views, will allow for major advances in these areas. This will be accomplished by innovative development of a novel iterative deep learning and dictionary learning approach that utilizes imaging physics such that limited data is required to train the network to perform tomographic reconstructions (i.e. 10s of views rather than 100-1000s). This approach represents a fundamental advancement in the ability to perform learning with training. These two aspects of our reconstruction algorithm represent major advances that can propel Los Alamos to the forefront of limited view tomography.

Technical Outcomes

The team developed a patched based generative adversarial network hat allows for the accurate reconstruction of complex objects for both extremely limited numbers of views (4) as well as very small data sets (1). We are currently, utilizing the technology to examine the feasibility of extending the radiographic capability of the hydrodynamic program at Los Alamos as well as utilizing this capability to make ground breaking advances in the emergency response community.

Publications

Conference Papers

Klasky, M. L., A. Lahiri, J. Fessler and S. Ravishankar. Limited-view Cone Beam CT reconstruction using 3D Patch-based Supervised and Adversarial Learning. Presented at *OSA Digital Holography and Three-Dimensional Imaging Topical Meeting (DH)*. (Vancover, Canada, 2021-07-19 - 2021-07-23). (LA-UR-21-22227)

Klasky, M. L., L. A. Pfister, J. L. S. Disterhaupt, M. T. McCann and S. Ravishankar. Descattering and Reconstruction in MultiMaterial Polyenergetic X-Ray Tomography Using Local Scatter Models. Presented at *OSA Digital Holography and Three-Dimensional Imaging Topical Meeting (DH)*. (Vancouver, Canada, 2021-07-19 - 2021-07-19). (LA-UR-21-22245)

Presentation Slides

Klasky, M. L., M. T. McCann, B. E. Wohlberg, M. Hossain, D. L. Sanzo, J. L. S. Disterhaupt, M. A. Espy, O. Korobkin, B. M. Patterson, T. Wilcox, A. Lahiri, J. Fessler, C. Bouman and S. Ravishankar. Dynamic Imaging: Beyond the Standard Model. Presented at *T-Division Student Talk*, Los Alamos, New Mexico, United States, 2021-07-22 - 2021-07-22. (LA-UR-21-27913)

Klasky, M. L., M. T. McCann, M. Hossain, D. L. Sanzo, J. L. S. Disterhaupt, O. Korobkin, T. Wilcox, J. W. Burby, S. Majee, A. Lahiri, J. Fessler, C. Bouman and S. Ravishankar. Coupled Hydrodynamic/Radiographic Dynamic Reconstructions: Beyond the Standard Model. Presented at *Enabling 3D mesoscale imaging under dynamic conditions*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-29231)

Klasky, M. L., S. Ravishankar, A. Lahiri and J. Fessler. Limited-view Cone Beam CT reconstruction using 3D Patch-based Supervised and Adversarial Learning. Presented at *Dynamic Radiography*, Los Alamos, New Mexico, United States, 2021-04-05 - 2021-04-05. (LA-UR-21-23792)

Lahiri, A., S. Ravishankar, M. L. Klasky and J. Fessler. Limited-View Cone Beam CT Reconstructions using 3D Patch Based Supervised and Adversarial Learning. Presented at *OSA Digital Holography and Three-Dimensional Imaging Topical Meeting*, Vancouver, Canada, 2021-07-26 - 2021-07-26. (LA-UR-21-27545)

Closing the Loop: Real-Time Neuromorphic Agents

Garrett Kenyon
20210758ER

Project Description

The next generation of machine learning algorithms must be able to learn in an unsupervised manner without undue reliance on human-provided labels but by interacting with their environments as self-organizing agents in a closed-loop feedback system. Our objective in this project is to construct just such an agent using neuromorphic components trained in an unsupervised manner using local, biologically plausible synaptic plasticity rules. Biologically-derived self-organizing capabilities will be complemented with global reward signals to accomplish specific tasks via well-established reinforcement learning (RL) techniques. We ultimately aim to demonstrate a biomimetic visual system constructed entirely from light-weight, low-power neuromorphic elements that can learn to search for and identify targets in natural environments. If successful, the reserve project will take an important step toward true machine intelligence.

Technical Outcomes

The team investigated approaches for training neuromorphic processors in an unsupervised manner using local, biologically plausible synaptic plasticity rules in a manner intended to mimic how humans and other animals learn during infant development. First, the team sought to verify that lateral competition between spiking neurons on a neuromorphic processor would function similarly to lateral competition between identically coupled non-spiking neurons. Results indicate that while both networks behaved similarly there were significant differences.

Publications

Journal Articles

Henke, K. G., G. Kenyon and B. J. Migliori. Fast Post-Hoc Normalization for Brain Inspired Sparse Coding on a Neuromorphic Device. Submitted to *IEEE Transactions on Parallel and Distributed Systems*. (LA-UR-21-22149)

Posters

Henke, K. G., G. Kenyon and B. J. Migliori. Brain Inspired Quantum and Neuromorphic Machine Learning. Presented at *NAML Workshop 2021*, Albuquerque, New Mexico, United States, 2021-03-23 - 2021-03-25. (LA-UR-21-22148)

Automatic Colormap Improvement in non-Euclidean Spaces

Roxana Bujack
20200512ECR

Project Description

The results of this project can help all application scientists. They depend on scientific visualization for the analysis of their experiments and simulations, for validation and verification and for gaining insight. At Los Alamos, these insights evolve into mission relevant conclusions that are communicated to stakeholders. Colormapping is one of the most common methods to visualize data. A poor colormap hides details or introduces artifacts; a good colormap promotes insight and communication. This project's goal is to extend the interactive Charting Continuous Colormap (CCC) tool (https://ccctool.com) to allow a user to correct and adjust a colormap. This will enable scientists to quickly generate high quality but also customized colormaps. That means that the colormaps will satisfy the specific needs of the scientists, for example, domain conventions, or color constraints due to annotations. At the same time, they will be comparable in quality to carefully designed high quality colormaps.

Publications

Journal Articles

Bujack, R. B., E. N. Stark, J. M. Miller, E. Caffrey and T. Turton. Perceptual Color Space is Riemannian, or is it?. Submitted to *Nature*. (LA-UR-21-24630)

Miller, J. M. and R. B. Bujack. Navigating the Gargantua System: Minimal Geodesic Curvature Paths and the Relativistic Transfer. Submitted to *Classical and Quantum Gravity*. (LA-UR-21-24971)

Teti, E. S., T. Turton, J. M. Miller, S. Hong, E. Barenholtz and R. B. Bujack. Validation of Crowdsourced Experiments for Color Perception. Submitted to *Psychological Methods*. (LA-UR-22-22545)

Teti, E. S., T. Turton, J. M. Miller and R. B. Bujack. Maximum Likelihood Estimation of Difference Scaling Functions for Suprathreshold Judgments. Submitted to *Journal of Vision*. (LA-UR-21-31281)

Conference Papers

Bujack, R. B., E. Caffrey, E. N. Stark, T. Turton and J. M. Miller. Efficient Computation of Geodesics in Color Space. Presented at *IEEE Vis*. (oklahoma city, Oklahoma, United States, 2023-10-16 - 2023-10-16). (LA-UR-21-24634)

Nardini, P. A., M. Chen, M. Boettinger, G. Scheuermann and R. B. Bujack. Automatic Improvement of Continuous Colormaps in Euclidean Colorspaces. Presented at *EuroVis*. (zurich, Switzerland, 2021-06-14 - 2021-06-14). (LA-UR-19-29080)

Nardini, P. A., M. Chen, R. B. Bujack, M. Boettinger and G. Scheuermann. A Testing Environment for Continuous Colormaps. Presented at *IEEE VIs*. (Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25). (LA-UR-20-22115)

Reports

Bujack, R. B. Grok Color. Unpublished report. (LA-UR-20-25476)

Bujack, R. B. Visualization Showcases. Unpublished report. (LA-UR-21-29064)

Bujack, R. B., N. W. Birge, V. Geppert-Kleinrath, P. L. Volegov and D. H. Rogers. Topological Analysis for Fusion Ignition. Unpublished report. (LA-UR-21-29431)

Stark, E. N., T. Turton, J. M. Miller and R. B. Bujack. Modeling Color Perception without Assuming Additivity of Color Differences. Unpublished report. (LA-UR-21-24906)

Presentation Slides

Stark, E. N. Diminishing Returns in Color Perception Dissertation Prospectus. . (LA-UR-21-23767)

Teti, E. S. Robotic Olfaction, Human Color Perception, and X-ray Emission Spectroscopy: Victims of "Unfortunate Data". . (LA-UR-21-30342)

Teti, E. S. Diminishing Returns in Color Perception. . (LA-UR-22-21695)

Other

Bujack, R. B. Geodesics in Color Space. Dataset. (LA-UR-21-22239)

Bujack, R. B., E. S. Teti, J. M. Miller, E. Caffrey and T. Turton.
  Empirical Data from Judgments of Achromatic Color
  Differences. Dataset. (LA-UR-22-20256)

Enhancing Bayesian Multivariate Adaptive Regression Spline Models Using Concepts from Deep Learning

Devin Francom
20200571ECR

Project Description

Machine learning is an important tool in the National Nuclear Security Administration (NNSA) arsenal for addressing many national security challenges, though it has blatant failures. The goal of this project is to combine concepts from the most successful machine learning algorithms with more principled statistical learning models to get accurate, interpretable, and robust new machine learning models that can be trusted in a wider set of circumstances. The potential is for these new models to be useful where other machine learning methods have failed, including some key NNSA mission areas with sparse datasets.

Publications

Journal Articles

Collins, G. Q., D. C. Francom and K. N. Rumsey. Bayesian Projection Pursuit Regression. Submitted to *Bayesian Analysis*. (LA-UR-22-21174)

Francom, D. C., B. Sanso and A. Kupresanin. Landmark-Warped Emulators for Models with Misaligned Functional Response. 2022. *SIAM/ASA Journal on Uncertainty Quantification*. **10** (1): 125-150. (LA-UR-21-30482 DOI: 10.1137/20M135279X)

Rumsey, K. N., D. C. Francom and A. A. Shen. Generalized Bayesian MARS: Robust, Quantile and Flexible-Likelihood Regression. Submitted to *Journal of the American Statistical Association*. (LA-UR-21-20776)

Reports

Shen, A. A., K. N. Rumsey and D. C. Francom. TBASS: A Robust Adaptation of Bayesian Adaptive Spline Surfaces. Unpublished report. (LA-UR-20-27873)

Presentation Slides

Francom, D. C. Bayesian MARS for efficient and informative nonlinear regression. Presented at *Quality and Productivity Research Conference*, Tallahassee, Florida, United States, 2021-07-26 - 2021-07-26. (LA-UR-21-27269)

Shen, A. A., D. C. Francom and K. N. Rumsey. Robust Bayesian Multivariate Adaptive Regression Splines (BMARS). . (LA-UR-20-27874)

Differentiable Programming: Bridging the Gap between Numerical Models and Machine Learning Models

Daniel O'Malley
20200575ECR

Project Description

Many national security problems involve components where physical laws are well-understood and other components where the physical laws are either poorly understood or not applicable. Traditional physical models excel at the former whereas interpolating data with machine learning (ML) excels at the latter, but neither approach can tackle these components simultaneously. Existing ML approaches to handling these types of components simultaneously are minor tweaks to standard ML methods. Tweaking black-box ML models is fundamentally limited because "big data does not interpret itself"–meaningful, interpretable structure in models is a necessity to improve predictability, enable human understanding, and maximize the impact of small data. We will meld trustworthy numerical modeling with trainable ML to produce fast models that can thrive on small data through an emerging technology called Differentiable Programming (DP). This project will harness DP to develop cutting-edge computational models of complex physics phenomena critical to national security. Through two applications, we will demonstrate that DP allows us to leverage rigorous physical models in the new paradigm of artificial intelligence (AI)-based science that is being vigorously pursued by Department of Energy (DOE).

Publications

Journal Articles

Greer, S. Y., J. D. Hyman and D. O'Malley. A Comparison of Linear Solvers for Resolving Flow in Three-Dimensional Discrete Fracture Networks. Submitted to *Water Resources Research*. (LA-UR-21-28243)

*Harp, D. R., D. O'Malley, B. Yan and R. J. Pawar. On the feasibility of using physics-informed machine learning for underground reservoir pressure management. 2021. *Expert Systems with Applications*. 115006. (LA-UR-21-20260 DOI: 10.1016/j.eswa.2021.115006)

Kadeethum, T., D. O'Malley, J. N. Fuhg, Y. Choi, J. Lee, H. S. Viswanathan and N. Bouklas. A framework for data-driven solution and parameter estimation of PDEs using conditional generative adversarial networks. Submitted to *Nature Computational Science*. (LA-UR-21-24958)

Kadeethum, T., F. Ballarin, Y. Choi, D. O'Malley, H. Yoon and N. Bouklas. Non-intrusive reduced order modeling of natural convection in porous media using convolutional autoencoders: comparison with linear subspace techniques. Submitted to *Advances in Water Resources*. (LA-UR-21-26841)

Wu, H., D. O'Malley, J. K. Golden and V. V. Vesselinov. Learning to regularize with a variational autoencoder for hydrogeologic inverse analysis. Submitted to *Advances in Water Resources*. (LA-UR-21-25990)

Presentation Slides

Kadeethum, T., F. Ballarin, Y. Choi, D. O'Malley, H. Yoon and N. Bouklas. Data-driven solution of natural convection in porous media. Presented at *InterPore*, Online, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25113)

O'Malley, D. Differentiable Programming: Bridging the gap between numerical models and machine learning models. Presented at *Computational Methods in Water Resources*, Online, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30090)

O'Malley, D. Differentiable Programming: Bridging the Gap Between Numerical Models and Machine Learning Models. Presented at *SIAM Geosciences*, Online, New Mexico, United States, 2021-06-21 - 2021-06-21. (LA-UR-21-25809)

O'Malley, D. Differentiable Programming: Bridging the gap between numerical models and machine learning models. Presented at *Machine Learning in Solid Earth Geoscience Lecture*, Online, New Mexico, United States, 2021-10-08 - 2021-10-08. (LA-UR-21-30196)

O'Malley, D. Differentiable Programming: Bridging the gap between numerical models and machine learning models. . (LA-UR-21-31190)

O'Malley, D. PDE constrained optimization and AI. Presented at *Meeting between LANL and AI4Opt*, Online, New Mexico, United States, 2022-02-03 - 2022-02-03. (LA-UR-22-20916)

Wu, H., D. O'Malley, J. K. Golden and V. V. Vesselinov. Regularization with a variational autoencoder for hydrogeologic inverse analysis. Presented at *Geological Society of America Annual Meeting 2021*, virtual, Oregon, United States, 2021-10-10 - 2021-10-13. (LA-UR-21-29280)

Distributed Algorithms for Large-Scale Ordinary Differential/Partial Differential Equation (ODE/PDE) Constrained Optimization Problems on Graphs

Kaarthik Sundar
20200603ECR

Project Description

Analysis of critical infrastructure (natural gas, water, etc.) is a very important national security challenge. The socio-economic systems of the United States depend on the reliable delivery of energy, water, etc. in order to function. As a result, the Department of Energy (DOE) and other stakeholders are tasked with ensuring these systems are safe and robust. However, the ability of policy makers to analyze and protect these systems is limited by the computational requirements of solving related problems in these systems at a nation-wide scale. This project is focused squarely on building the fundamental algorithms that reduce these computational burdens and facilitate the ability of policy makers to make informed decisions on how to best secure the nation's critical infrastructure.

Publications

Journal Articles

Misra, S., K. Sundar, R. Sharma and K. Brink. Deployable, Data-Driven Unmanned Vehicle Navigation System in GPS-Denied, Feature-Deficient Environments. Submitted to *Journal of Intelligent and Robotic Systems*. (LA-UR-21-20249)

Rajan, S., K. Sundar and N. Gautam. Routing problem for Unmanned Aerial Vehicle patrolling missions—A progressive hedging algorithm. 2022. *Computers & Operations Research*. 105702. (LA-UR-21-24769 DOI: 10.1016/j.cor.2022.105702)

Sundar, K., S. Sanjeevi and H. Nagarajan. Sequence of Polyhedral Relaxations for Nonlinear Univariate Functions. Submitted to *Optimization and Engineering*. (LA-UR-20-23980)

Sundar, K. and S. Sanjeevi. A Branch-and-Price Algorithm for a Team Orienteering Problem for Fixed-Wing Drones. Submitted to *EURO Journal on Transportation and Logistics*. (LA-UR-19-32483)

Conference Papers

Shin, S., C. J. Coffrin, K. Sundar and V. M. Zavala. Graph-Based Modeling and Decomposition of Energy Infrastructures. Presented at *11th IFAC SYMPOSIUM on Advanced Control of Chemical Processes*. (Venice, Italy, 2021-06-13 - 2021-06-16). (LA-UR-20-27539)

Quantum Information-Based Complexity

Yigit Subasi
20210639ECR

Project Description

Developing simulation capabilities and deploying computing platforms to analyze and predict the performance, safety, and reliability of nuclear weapons became essential since physical nuclear tests have been banned. Given the extraordinary complexity of nuclear weapons systems there is a need for very large scale modeling and simulation and the computational resources grow exponentially. A similar problem is encountered when studying quantum matter; even the simulation of microscopic molecules can be beyond the reach of supercomputers. Quantum computers promise to solve some problems more efficiently than any classical computer can. Unfortunately, identifying such problems has proven hard and a quantum speed up has been shown only for a small number of problems. In this project we will develop a theoretical framework that will enable us to analyze the quantum complexity of problems and develop efficient algorithms for solving them. In particular, our proposed formalism and tools will help rule out problems with no possibility of quantum advantage. By doing so, they will guide research efforts towards fruitful directions.

Publications

Journal Articles

Holmes, Z. P., N. J. Coble, A. T. Sornborger and Y. Subasi. On nonlinear transformations in quantum computation. Submitted to *Quantum*. (LA-UR-21-32322)

Volkoff, T. J. and Y. Subasi. Ancilla-free continuous-variable SWAP test. Submitted to *Quantum*. (LA-UR-22-21141)

Presentation Slides

Schoute, E., M. Beverland and V. Kliuchnikov. Surface code compilation via edge-disjoint paths. Presented at *Quantum Science Center*, College Park, Maryland, United States, 2022-02-02 - 2022-02-02. (LA-UR-22-20684)

Posters

Beverland, M., V. Kliuchnikov and E. Schoute. Surface code compilation via edge-disjoint paths. Presented at *Quantum Information Processing 2022*, Pasadena, California, United States, 2022-03-07 - 2022-03-07. (LA-UR-22-21915)

Accelerated Monte Carlo Algorithms without Detailed Balance

Ying Wai Li
20210662ECR

Project Description

The project will develop smart, efficient, and parallel stochastic methods for computer simulations that are readily scalable on leadership-class supercomputers. The Monte Carlo (MC) algorithms to be developed in this work are a fundamental tool in computational physics that has a tremendous range of mission-relevant applications across Los Alamos National Laboratory (LANL), National Nuclear Security Administration (NNSA), and Department of Energy (DOE). MC enables the study of neutron and radiation transport and defect dynamics in materials at the mesoscale, making MC methods the workhorses for studying nuclear physics, high energy physics, matter phases, transitions, and aging, as well as equilibrium and non-equilibrium phenomena. Improved MC methods can greatly benefit scientific machine learning, uncertainty quantification, and emulation of quantum computers. General improvements to MC methodology proposed in this work could greatly benefit all of these fields. Moreover, MC methods are naturally suitable for advanced parallel computer hardware such as many-core processors and graphics processing unit (GPU) accelerators, so successful execution of this work will reduce the time-to-solution for solving scientific grand challenges on the DOE's leadership-class supercomputers.

Publications

Journal Articles

Ferreira, T., S. R. Acharya, Y. W. Li, D. Parker, A. S. Sefat and V. R. Cooper. Unintended Consequence of Topochemical Reduction of $SrFeO_3$ to $SrFeO_2$: Design of Infinite Layered-Oxides. 2021. *Physical Review Materials*. **5** (12): 123401. (LA-UR-21-27840 DOI: 10.1103/PhysRevMaterials.5.123401)

Presentation Slides

Li, Y. W. Machine Learning Assisted Simulations of Materials Thermodynamics. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-28 - 2022-03-03. (LA-UR-22-21946)

Li, Y. W. and T. Vogel. Accelerating Multicanonical Sampling with Irreversibility. Presented at *35th Annual CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens (Virtual), Georgia, United States, 2022-02-21 - 2022-02-24. (LA-UR-22-22032)

Posters

Sattar, N. S. and Y. W. Li. Accelerating Parallel Monte Carlo Simulations for Statistical Physics: Portability on Many-Core Processors. Presented at *Supercomputing 21*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-19. (LA-UR-21-28319)

Statistical Learning for Field Theories

Andrey Lokhov
20210674ECR

Project Description

Field theories lie at the heart of modern natural sciences, with a wide range of interdisciplinary applications ranging from classical electrodynamics or gravitation, through statistical physics or turbulent flows, to condensed matter or high energy physics. Non-linearities of interactions in non-trivial field theories typically preclude analytic precise predictions within these models even when the underlying physics is well understood. Radically new ideas for validating field theory models are required for making progress in non-linear science in the twenty-first century. The goals of this proposal are two-fold: first, development of novel methods for learning of field theories from scarce experimental measurements or data obtained from costly first-principles simulations; second, demonstration of our central hypothesis that even those field theories for which generation of quantitative predictions is intractable can be still be validated using a novel statistical-learning based method. If successful, the proposed research will likely produce a substantial impact on the modern theory of high-energy, condensed matter, and turbulence physics which are among the priority research directions for Los Alamos National Laboratory (LANL), leading to a new path towards non-perturbative methods in Quantum Field Theory and fluid dynamics and advancing the forefront of these fields.

Publications

Presentation Slides

Lokhov, A. Learning of classical lattice Hamiltonians. Presented at *Seminar at RPI*, Online, New Mexico, United States, 2021-10-27 - 2021-10-27. (LA-UR-21-30704)

Numerical Methods for Radiation Hydrodynamics Simulations on Current and Future Advanced Parallel Architectures

Jonas Lippuner
20190519ECR

Project Description

To ensure the safety and reliability of the United States nuclear stockpile, large-scale, sophisticated, multi-physics computer simulations of nuclear explosions are necessary since the US does not conduct nuclear tests anymore. To perform these simulations, the Department of Energy operates the largest supercomputers in the world. The computing hardware in these supercomputers has changed dramatically in the last decade and most of the computing power (up to 95%) is now in special, advanced architecture chips, such as graphics processing units (GPUs). The simulation codes used today were designed long before these chips were invented and the methods and algorithms used in our codes are not necessarily the best suited ones for the current and future hardware. This project seeks to investigate which methods perform most efficiently on this advanced hardware and to develop new such methods. The results of this work will be crucial to decide the future direction of the various programmatic simulation code development efforts of the National Nuclear Security Administration. The new methods developed as part of this project will also help ensure that our large-scale physics simulations run efficiently on current and future supercomputers.

Technical Outcomes

The project resulted in the development of Ethon, a software framework to study hydrodynamics methods with block-based adaptive mesh refinement on different computing architectures. Ethon was released to the public as open source software. Ethon demonstrated a speed up of 4x to 7x on graphics processing units compared to traditional multi-core central processing units. Ethon can now be used by the community to investigate the performance of different numerical methods on various computing architectures.

Publications

Journal Articles

*Fernandez, R., F. Foucart and J. Lippuner. The landscape of disc outflows from black hole–neutron star mergers. 2020. *Monthly Notices of the Royal Astronomical Society*. **497** (3): 3221-3233. (LA-UR-20-23877 DOI: 10.1093/mnras/staa2209)

Lippuner, J. Ethon: A software framework for hydrodynamics simulations with block-based AMR on parallel computing architectures. Submitted to *SoftwareX*. (LA-UR-21-20255)

Reports

Lippuner, J. Ethon hydrodynamics notes. Unpublished report. (LA-UR-20-30347)

Improving Predictions of Complex Systems with Predictive Discrepancy Models and Data Fusion

David Osthus
20190546ECR

Project Description

Disease spread represents a vulnerability and risk to our national security. Pandemics don't respect borders and pose a significant burden on our populace and infrastructure. Intervention strategies are only successful if deployed in a timely, efficient, and targeted manner. Preferably, interventions are proactive rather than reactive. Before we can proactively counter disease spread, however, we have to be able to forecast its spread. Thus, disease forecasting capabilities constitute a significant link in the national security chain. This project will develop state, regional, and national flu forecasting models that will be deployed in real-time to maximize impact with public health decision makers. These models will push the limits of disease forecasting by bringing together state-of-the-art mathematical modeling with numerous data sources. The mathematical modeling advances are relevant to many applications with incomplete theory, experimental data, and the need to make predictions with quantified uncertainties. As such, this work has broad applicability to Department of Energy and National Nuclear Security Administration applications, such as nuclear weapons, nonproliferation, and energy, as well as direct applications in National Institutes of Health and Centers for Disease Control and Prevention.

Technical Outcomes

This project developed the first multiscale influenza forecasting model in the United States. The model, called Dante, participated in and won the U.S. Centers for Disease Control and Preventions flu forecasting challenge in 2018/19. Dante was made much faster with a new model, Inferno. The work developed in this project has been extended to both Coronavirus (COVID-19) forecasting as well as space weather forecasting.

Publications

Journal Articles

Cramer, E., Y. Huang, Y. Wang, E. Ray, M. Cornell, J. Bracher, A. Brennen, A. Castero Rivadeneira, A. Gerding, T. Gneiting, K. House, D. Jayawardena, A. Hannan Kanji, A. Khandelwal, K. Le, A. Muhlemann, J. Niemi, A. Stark, A. Shah, N. Wattanchit, M. Zorn, D. A. Osthus, L. A. Castro, I. J. Michaud, G. Fairchild and N. Reich. The United States COVID-19 Forecast Hub dataset. Submitted to *Scientific Data - Nature*. (LA-UR-21-29146)

Gibson, G. C., D. A. Osthus, K. R. Moran and N. G. Reich. Improving Probabilistic Infectious Disease Forecasting Through Coherence. Submitted to *PLOS Computational Biology*. (LA-UR-19-32598)

Osthus, D. A. Fast and Accurate Influenza Forecasting in the United States with Inferno. Submitted to *PLOS Computational Biology*. (LA-UR-20-30384)

*Osthus, D. A. and K. R. Moran. Multiscale influenza forecasting. 2021. *Nature Communications*. **12** (1): 2991. (LA-UR-19-28977 DOI: 10.1038/s41467-021-23234-5)

Picard, R. R. and D. A. Osthus. Forecast Intervals for Infectious Disease Models. Submitted to *International Journal of Forecasting*. (LA-UR-20-29644)

Shelley, C. D., G. Rajasekar, M. K. Lieng and M. Nu\xc3\xb1o. Characteristics and Severity of COVID-19 Patients in Five Academic Hospitals in California. Submitted to *Journal of Epidemiology & Community Health*. (LA-UR-21-20303)

Presentation Slides

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

Castro, L. A. and C. D. Shelley. Leveraging a COVID-19 Case Forecasting Model for Predicting Health Care Needs in New Mexico: A Quantitative Analysis. . (LA-UR-21-20636)

Osthus, D. A. Dante: An Applied Statistician's Approach to Flu Forecasting. Presented at *FluSight Seasonal Influenza Forecasting Workshop*, Atlanta, Georgia, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28213)

Osthus, D. A. Dante: An Applied Statistician's Approach to Flu Forecasting. . (LA-UR-19-28798)

Osthus, D. A. What we've learned from 7 years of real-time flu forecasting in the United States. Presented at *Joint Statistical Meetings*, Online, New Mexico, United States, 2020-08-02 - 2020-08-02. (LA-UR-20-25785)

Osthus, D. A. and K. R. Moran. Multiscale Flu Forecasting. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-28 - 2019-07-28. (LA-UR-19-27237)

Posters

Osthus, D. A. 2018/19 FluSight Challenge Dante and DBM +. Presented at *FluSight Seasonal Influenza Forecasting Workshop*, Atlanta, Georgia, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28198)

Optimizing Scientific Codes in the Presence of Extreme Heterogeneity Using Machine Learning

Eun Jung Park
20190566ECR

Project Description

Existing hint-based approaches to optimizing the translation of human code to machine code for complex scientific codes have been effective at generating efficient code for traditional architectures, but emerging heterogeneous architectures have proven too complex for existing techniques. This project will leverage emerging machine learning techniques to perform code translation for complex, heterogeneous machine architectures. The resulting techniques will be one critical step in supporting scientific computing on the non-traditional computer architectures expected to replace existing supercomputing platforms in the post-Exascale era.

Technical Outcomes

The project successfully constructed machine learning models by correlating architecture and application features to predict effective order of compiler optimizations in compilers. The project introduced novel features including data utilization rate and graph-based application features and also advanced existing graph-based learning methods for better application to compiler optimization problems. The resulting techniques/framework provide an important step, enabling the application of current ML-based techniques to improve Department of Energy applications and construct more intelligent compiler frameworks.

Publications

Conference Papers

Jayatilaka, T., H. Ueno, J. Doerfert, E. J. Park and G. Georgakoudis. Towards Compile-Time-Reducing Compiler Optimization Selection via Machine Learning. Presented at *ML for Computer Architecture and Systems*. (Virtual, New Mexico, United States, 2021-06-14 - 2021-06-19). (LA-UR-21-24916)

Discrete Optimization Algorithms for Provably Optimal Quantum Circuit Design

Harsha Nagarajan
20190590ECR

Project Description

As stated in the 2018 United States national strategic overview for Quantum Information Science (QIS), "QIS applies the best understanding of the sub-atomic world—quantum theory—to generate new knowledge and technologies. Prior applications of QIS-related technologies include semiconductor microelectronics, the global positioning system (GPS), and magnetic resonance imaging (MRI). These also underpin significant parts of the national economic and defense infrastructure". QIS, applied in quantum computers, has the potential to dramatically outperform classical computers. Research and development in QIS is one of the the Department of Energy's growth areas. This project is focused squarely on building the fundamental algorithms that reduce the computational burden and provide new design architectures that facilitate the ability of DOE policy makers to make informed decisions on the design of next-generation quantum computers. The algorithms developed in this project will have a direct impact on the Laboratory's research missions. Also, due to the fundamental nature of this project, it will build underlying capability with likely future applicability to DOE Office of Electricity (OE) needs such as the "Networked Microgrids" and "Resilient Design Tool for Distribution Networks" projects.

Technical Outcomes

Towards chasing the overarching goal of quantum supremacy, the goal of this project was to decompose an arbitrary entangled state, represented as a unitary, in to a sequence of gates supported by a quantum processor (up to a global phase and machine precision) by minimizing the noisy controlled NOT (CNOT) gates. This project successfully explored rigorous discrete optimization-based methods, via efficiently formulated mixed-integer programs, to accelerate numerically provable optimal quantum circuits and released Julia-based "QuantumCircuitOpt", an open-source framework.

Publications

Journal Articles

Bhela, S., H. Nagarajan, D. Deka and V. Kekatos. Efficient Topology Design Algorithms for Power Grid Stability. Submitted to *IEEE Control Systems Letters*. (LA-UR-21-22364)

Ryu, M., H. Nagarajan and R. W. Bent. Mitigating the Impacts of Uncertain Geomagnetic Disturbances on Electric Grids: A Distributionally Robust Optimization Approach. Submitted to *IEEE Transactions on Power Systems*. (LA-UR-21-22568)

Conference Papers

Nagarajan, H., O. Lockwood and C. J. Coffrin. QuantumCircuitOpt: An Open-source Framework for Provably Optimal Quantum Circuit Design. Presented at *SC21: The International Conference for High Performance Computing, Networking, Storage, and Analysis*. (St Louis, Missouri, United States, 2021-11-14 - 2021-11-19). (LA-UR-21-30795)

Other

Nagarajan, H., O. Lockwood and C. J. Coffrin. QuantumCircuitOpt: An Open-source Framework for Provably Optimal Quantum Circuit Design. Audio/Visual. (LA-UR-21-31731)

Emergent Quantum Phenomena with Tensor Networks

Lukasz Cincio
20190659PRD4

Project Description

The development of quantum computers is crucial for the national security. It requires novel materials and insights into the fundamental properties of quantum systems, which frequently require new numerical methods. The goal of this research is to develop such methods and apply them to materials that may open path to noise resilient topological quantum computation and to fundamental limitations on adiabatic quantum computation used by the D-Wave quantum computer.

Publications

Journal Articles

Cincio, L., D. Bultrini, M. E. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith and P. J. Coles. Unifying and benchmarking state-of-the-art quantum error mitigation techniques. Submitted to *Quantum*. (LA-UR-21-27288)

A. A. *. C. P. J. *. C. L. Czarnik, P. *., P. J. Coles, L. Cincio, P. Czarnik and A. Arrasmith. Error mitigation with Clifford quantum-circuit data. 2021. *Quantum*. **5**: 592. (LA-UR-20-23755 DOI: 10.22331/q-2021-11-26-592)

Czarnik, P. J., A. T. Arrasmith, L. Cincio and P. J. Coles. Qubit-efficient exponential suppression of errors. Submitted to *arXiv+PRX Quantum*. (LA-UR-21-21151)

*Czarnik, P., M. M. Rams, P. Corboz and J. Dziarmaga. Tensor network study of the m = 1/2 magnetization plateau in the Shastry-Sutherland model at finite temperature. 2021. *Physical Review B*. **103** (7): 075113. (LA-UR-20-29946 DOI: 10.1103/PhysRevB.103.075113)

LaRose, R., A. Mari, S. Kaiser, P. J. Kralekas, A. A. Alves, P. J. Czarnik, M. El Mandouh, M. H. Gordon, Y. Hindy, A. Robertson, P. Thakre, N. Shammah and W. J. Zeng. Mitiq: A software package for error mitigation on noisy quantum computers. Submitted to *arXiv*. (LA-UR-21-25925)

Larocca, M., P. J. Czarnik, K. Sharma, G. Muraleedharan, P. J. Coles and M. V. S. Cerezo de la Roca. Diagnosing barren plateaus with tools from quantum optimal control. Submitted to *Physical Review X Quantum*. (LA-UR-21-24973)

*Lowe, A., M. H. Gordon, P. Czarnik, A. Arrasmith, P. J. Coles and L. Cincio. Unified approach to data-driven quantum error mitigation. 2021. *Physical Review Research*. **3** (3): 033098. (LA-UR-20-28845 DOI: 10.1103/PhysRevResearch.3.033098)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, P. J. Czarnik, L. Cincio and P. J. Coles. Effect of barren plateaus on gradient-free optimization. Submitted to *Quantum*. (LA-UR-20-29699)

Wang, S., P. J. Coles, P. J. Czarnik, A. T. Arrasmith, M. V. S. Cerezo de la Roca and L. Cincio. Can Error Mitigation Improve Trainability of Noisy Variational Quantum Algorithms?. Submitted to *Physical Review X, arxiv.org*. (LA-UR-21-28574)

Reports

Cincio, L. Error mitigation with Clifford quantum-circuit data. Unpublished report. (LA-UR-22-21698)

Presentation Slides

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Czarnik, P. J. Tensor network simulation of two-dimensional strongly correlated systems. Presented at *IonQ seminar*, College Park, Maryland, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-21998)

Czarnik, P. J., A. Lowe, M. H. Gordon, A. T. Arrasmith, P. J. Coles and L. Cincio. Data-driven error mitigation for near-term quantum computers. Presented at *Seminar of Institute of Theoretical Physics of Jagiellonian University, Cracow*, Cracow, Poland, 2020-12-10 - 2020-12-10. (LA-UR-20-30043)

Czarnik, P. J., A. Lowe, M. H. Gordon, A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation for gate-based quantum computers. Presented at *IonQ seminar*, College Park, Maryland, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-22055)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *Quantum Information Processing*, Munich, Germany, 2021-02-01 - 2021-02-05. (LA-UR-21-20721)

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at

APS March Meeting, virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22444)

Lowe, A., M. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, P. J. Coles and L. Cincio. Unified Approach to Data Driven Quantum Error Mitigation. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22591)

Posters

Czarnik, P. J., A. T. Arrasmith, P. J. Coles and L. Cincio. Error mitigation with Clifford quantum-circuit data. Presented at *QuAlg20*, N/A (virtual), United Kingdom, 2020-09-22 - 2020-09-22. (LA-UR-20-27369)

Lowe, A., M. Hunter Gordon, P. J. Czarnik, A. T. Arrasmith, P. J. Coles and L. Cincio. Unified approach to data-driven quantum error mitigation. Presented at *Quantum Information Processing*, Online, New Mexico, United States, 2021-01-01 - 2021-01-05. (LA-UR-21-20496)

Other

Czarnik, P. J. Data from quantum many-body system calculations. Dataset. (LA-UR-22-21671)

Error Correction and Speed-up of Near-term Quantum Computing Architectures

Patrick Coles
20200677PRD1

Project Description

Quantum computation is an important facet of quantum technology, and constitutes a main focus of the National Quantum Initiative. Highly efficient quantum algorithms implemented in the settings of cryptography, distribution of quantum mechanical resources, and numerical optimization are vital for national information security in an age of quantum technology. The present project analyzes relationships between quantum computer architecture and the potential advantages that the quantum computer can provide, while maintaining an emphasis on near-term quantum devices, such as superconducting, photonic, and atomic quantum processors. This research is immediately applicable to proposed Department of Energy (DOE) missions that require quantum algorithms for enhanced computation and sensing. In particular, the project is focused on designing efficient quantum algorithm modules, which are necessary to exploit the advantages of both intermediate scale and large scale quantum computers.

Publications

Journal Articles

Pesah, A., M. V. S. Cerezo de la Roca, S. Wang, T. J. Volkoff, A. T. Sornborger and P. J. Coles. Absence of Barren Plateaus in Quantum Convolutional Neural Network. Submitted to *Physical Review X*. (LA-UR-20-29031)

*Tan, K. C. and T. Volkoff. Variational quantum algorithms to estimate rank, quantum entropies, fidelity, and Fisher information via purity minimization. 2021. *Physical Review Research*. **3** (3): 033251. (LA-UR-21-22998 DOI: 10.1103/PhysRevResearch.3.033251)

Volkoff, T. J. Efficient trainability of linear optical modules in quantum optical neural networks. Submitted to *arXiv*. (LA-UR-20-26436)

Volkoff, T. J. Distillation of maximally correlated bosonic matter from many-body quantum coherence. Submitted to *Quantum*. (LA-UR-20-27370)

Volkoff, T. J. Strategies for variational quantum compiling of a zero-phase beamsplitter on the Xanadu X8 processor. Submitted to *arXiv*. (LA-UR-22-20849)

Volkoff, T. J., Z. P. Holmes and A. T. Sornborger. Universal Compiling and (No-)Free-Lunch Theorems for Continuous-Variable Quantum Learning. 2021. *PRX Quantum*. **2** (4): 040327. (LA-UR-21-24060 DOI: 10.1103/PRXQuantum.2.040327)

Volkoff, T. J. and M. J. Martin. Asymptotic optimality of twist-untwist protocols for Heisenberg scaling in atom-based sensing. Submitted to *Physical Review Research*. (LA-UR-21-23486)

Volkoff, T. J. and Y. Subasi. Ancilla-free continuous-variable SWAP test. Submitted to *Quantum*. (LA-UR-22-21141)

*Volkoff, T. and P. J. Coles. Large gradients via correlation in random parameterized quantum circuits. 2021. *Quantum Science and Technology*. **6** (2): 025008. (LA-UR-20-23818 DOI: 10.1088/2058-9565/abd891)

Quantum Simulation of Quantum Field Theories

Rolando Somma
20200678PRD1

Project Description

This project studies foundational questions on the simulation of quantum field theories (QFTs), which describe the most fundamental particle interactions, with quantum computers. In contrast to standard computers, quantum computers are built upon quantum systems and exploit resources that would not be available otherwise. The expected outcomes are efficient quantum computational methods to study QFTs in regimes that are currently intractable, even for the largest supercomputers. A top quantum algorithms capability is essential for the Department of Energy and National Nuclear Security Administration to succeed in its quest to become world leaders in quantum information science. The results are expected to impact a number of missions including the National Quantum Initiative (NQI). The NQI Act calls for the establishment of a whole-of-Government approach to quantum information science.

Publications

Journal Articles

Sahinoglu, M. B., D. Williamson, N. Bultinck, M. Marien, J. Haegeman, N. Schuch and F. Verstraete. Characterizing topological order with matrix product operators. Submitted to *Annales Henri Poincare*. (LA-UR-20-29927)

Somma, R. D., M. B. Sahinoglu and S. Gu. Fast-forwarding quantum evolution. Submitted to *Quantum*. (LA-UR-20-29591)

Reports

Somma, R. D. and M. B. Sahinoglu. Complexity of product formulas in digital adiabatic state transformations. Unpublished report. (LA-UR-21-23267)

Presentation Slides

Sahinoglu, M. B. A tensor network framework for topological phases of quantum matter. Presented at *Mathematical Physics Days 2020*, Istanbul, Turkey, 2020-12-11 - 2020-12-13. (LA-UR-20-30131)

Sahinoglu, M. B. What is quantum information science? and How to be a quantum information scientist?. . (LA-UR-21-20600)

Sahinoglu, M. B. Error correction with tensor networks. Presented at *INT Program 21-1c: Tensor Networks in Many Body and Quantum Field Theory*, Seattle, Washington, United States, 2021-05-17 - 2021-06-04. (LA-UR-21-25022)

Sahinoglu, M. B. Quantum walks - an introduction. . (LA-UR-21-26393)

Sahinoglu, M. B. On two pillars of quantum computing: Fault tolerance and Hamiltonian simulation. . (LA-UR-21-27823)

Sahinoglu, M. B. and R. D. Somma. Hamiltonian simulation in the low energy subspace. . (LA-UR-20-27396)

In Situ Quantification of Damage in High Explosives

David Montgomery
20200744PRD1

Project Description

Understanding materials under extremes, their behavior under dynamic loading, contributions of defects to failure, and how high explosives remain safe under impact are important to Department of Energy/National Nuclear Security Administration missions for advanced material design and modeling materials with computers. Much of our understanding depends on defects in the materials, such as voids and cracks, and how those grow during an extreme event, such as impact. Three-dimensional (3-D) computed tomography, using hundreds of x-ray images from various angles, can measure such defects, but during a dynamic event there is only time for one or a few frames of x-ray images. Using advanced mathematical analysis techniques, prior knowledge of the types of defects, together with the physics of the x-ray image formation process, 3-D information about those defects can be obtained from a single x-ray image. This has been successfully applied to measuring lung alveoli in medical images and to voids in ceramics and will be applied to x-ray images of materials under dynamic loading taken with bright, laser-like x-ray sources in the United States. Such information will help inform and improve our computational models of crack growth and material failure important for security missions, including the nuclear weapons stockpile.

Publications

Presentation Slides

Leong, A. F. Characterizing the Dynamic Behavior of Porous Materials using X-ray Phase Contrast Imaging. Presented at *Physics Cafe (Virtual)*, Los Alamos, New Mexico, United States, 2021-07-22 - 2021-07-22. (LA-UR-21-27962)

Leong, A. F. Distribution measurement of micron-size features from XPCI images in the near-field to Fresnel regime. Presented at *Enabling 3D mesoscale imaging under dynamic conditions (Virtual)*, Los Alamos, New Mexico, United States, 2021-09-14 - 2021-09-16. (LA-UR-21-29033)

Pandolfi, S., A. Gleason, H. Lee, B. Nagler, E. Galtier, E. Cunningham, Y. Liu, S. Marchesini, K. Li, A. Sakdinawat, P. Hart, C. Curry, M. H. Seaberg, D. Khaghani, S. L. Vetter, F. J. Decker, W. Mao, T. Carver, R. Sandberg, D. S. Hodge, M. Ricks, C. McCombs, N. Blanchard, D. Montgomery, C. A. Bolme, P. M. Kozlowski, K. J. Ramos, M. S. Powell, A. F. Leong, S. Ali, P. Celliers, M. Dayton, L. Dresselhaus-Marais, T. Doeppner, L. D. Claus and M. O. Sanchez. Ultrafast time-resolved imaging of void collapse in ICF ablator materials. Presented at *APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-31420)

Posters

Montgomery, D., A. F. Leong, J. L. Barber, C. A. Bolme and K. J. Ramos. In situ phase contrast imaging for cracks and voids under dynamic loading. Presented at *2021 Conventional High Explosives Grand Challenge (CHEGC) Technical Symposium*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-10. (LA-UR-21-31792)

Addressing Data Challenges to Improve Prediction Models

Sara Del Valle
20210761PRD1

Project Description

Methodologies for fusing disparate data streams that can address sparse, misclassified, and missing data are critical for addressing many mission-relevant problems to address emerging and reemerging threats for the Nation. This project will do exactly that by developing approaches that can digest real-time data while correcting for their limitations to increase the reliability of models and forecasts.

Publications

Journal Articles

VanDervort, L. J. COVID-19 outcomes by cancer status, type, treatment, and vaccination. Submitted to *Journal of the National Cancer Institute*. (LA-UR-22-21557)

VanDervort, L. J., D. A. Osthus and S. Y. Del Valle. Addressing delayed case reporting in infectious disease forecast modeling. Submitted to *PLOS Computational Biology*. (LA-UR-21-30640)

VanDervort, L. J., P. Patelli, J. P. Schwenk, K. M. Martinez, T. R. Pitts, M. J. Barnard, K. A. Kaufeld, B. H. Mcmahon and S. Y. Del Valle. Multi-dimensional resilience: a quantitative exploration of disease outcomes and economic, political, and social resilience to the COVID-19 pandemic in six countries. Submitted to *PLOS One*. (LA-UR-21-31106)

Reports

VanDervort, L. J. Imputation of SARI Time Series. Unpublished report. (LA-UR-22-20223)

Presentation Slides

Osthus, D. A., L. J. VanDervort and S. Y. Del Valle. Addressing delayed case reporting for infectious disease models. . (LA-UR-21-27812)

VanDervort, L. J. Web Tool for Outcome Prognostication in Patients Newly-Diagnosed with Oropharyngeal Cancer. . (LA-UR-21-30661)

VanDervort, L. J. Measurement Error, Selection Bias, and Missing Data in Biomedical Research. Presented at *CCS-6 Seminar*, Los Alamos, New Mexico, United States, 2021-11-17 - 2021-11-17. (LA-UR-21-31246)

VanDervort, L. J. Statistics at Los Alamos National Laboratory. Presented at *Virtual Student seminar at University of Michigan Department of Biostatistics*, Ann Arbor, Michigan, United States, 2022-01-28 - 2022-01-28. (LA-UR-22-20528)

VanDervort, L. J. Primer on Ribbon Separation. . (LA-UR-22-20511)

VanDervort, L. J. Statistical inference for association studies using EHR: handling both selection bias and outcome misclassification. Presented at *University of Colorado Invited Seminar (Virtual)*, Los Alamos, New Mexico, United States, 2022-02-14 - 2022-02-14. (LA-UR-22-20963)

VanDervort, L. J., D. A. Osthus and S. Y. Del Valle. Addressing Data Challenges to Improve Prediction Models: Progress Update, Sept. 2021. . (LA-UR-21-29302)

Quantum Information with Atoms in Optical Tweezers

Michael Martin
20210955PRD3

Project Description

The subcommittee on Quantum Information Science under the Committee on Science of the National Science and Technology Council published a report in September 2018 entitled "National Strategic Overview for Quantum Information Science." Here, the economic and defense implications of quantum systems are discussed. Cited applications included optimization problems, chemistry, sensing, and machine learning. An outstanding challenge is to discover new systems and approaches that might one day impact these applications. Neutral atom systems, as developed here, are one promising approach, and sensing advantages may be imminent. This work will explore a system comprising interacting qubits encoded in individual neutral atoms, with a specific emphasis on an enabling technology: optical tweezers. First, we will develop a trapping strategy to elucidate the coherence and entanglement advantages of qubits stored in the nucleus of the alkaline earth atom strontium-87. Second, and in parallel, we will develop a robust method for entangling a single atom with a Bose-Einstein condensate sensor, which has the potential to increase sensor performance as well as explore fundamental questions relating to quantum correlations and entanglement.

AI-enabled Electron Dynamics at the Device Scale

Benjamin Nebgen
20210956PRD3

Project Description

The reduced computational cost of machine learning (ML) models for modeling electron dynamics would facilitate the simulation of million atom systems, allowing for first principles modeling of electron interactions with phonons, defects, surfaces and interfaces across entire devices. The computational framework will be inclusive of device complexities, for example, having solid-solid or solid-molecule interfaces and various types of defects. This will be useful for various projects central to Los Alamos National Laboratory's interest, e.g. energy conversion, bio-sensing, drug design and computation. Importantly, with the developed methodology will be critical for the formation of effective collaborations with researchers at Los Alamos (e.g. Center for Integrated nanotechnologies) whose work closely focus on two rapidly developing fields at the forefront of novel technologies: efficient plasmon driven hot carrier energy harvesting devices, and modeling the manipulation of electron spin states in promising materials for quantum computation and communication. For the broader scientific community, this device-scale electron dynamics will provide researchers the much-needed platform to understand the fundamental physical limitations present in the design of efficient technologies.

Publications

Journal Articles

Habib, A., R. Sundararaman, J. Xu, H. Takenaka and Y. Ping. Giant Spin Lifetime Anisotropy and Spin-Valley Locking in Silicene and Germanene from First-Principles Density-Matrix Dynamics. Submitted to *Nano Letters*. (LA-UR-21-30731)

Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches

Youzuo Lin
20210542MFR

Project Description

This project will build a capability in physics-informed machine learning, and will be poised for future subsurface energy & security programmatic efforts in carbon dioxide (CO2) sequestration, geothermal extraction, groundwater remediation, and underground nuclear-explosion monitoring, and the national security goal of energy security.

Publications

Journal Articles

Lin, Y., Q. Zeng, S. Feng and B. E. Wohlberg. InversionNet3D:High-Resolution 3D Full Waveform Inversion with Efficient Encoder-Decoder Network. Submitted to *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*. (LA-UR-21-22293)

Lin, Y., S. Feng, P. Jin and X. Zhang. Exploring Multi-physics with ExtremelyWeak Supervision. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-22-21115)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Connect the Dots: In Situ 4-D Seismic Monitoring of CO_2 Storage With Spatio-Temporal CNNs. 2021. *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-21-22295 DOI: 10.1109/TGRS.2021.3116618)

Lin, Y., S. Feng and B. E. Wohlberg. Multiscale Data-Driven Seismic Full-Waveform Inversion With Field Data Study. 2021. *IEEE Transactions on Geoscience and Remote Sensing*. (LA-UR-21-20004 DOI: 10.1109/TGRS.2021.3114101)

Lin, Y., Y. Feng, S. Feng, C. Deng, P. Jin and X. Zhang. OpenFWI: Benchmark Seismic Datasets for Machine Learning-Based Full Waveform Inversion. Submitted to *Geophysical Prospecting*. (LA-UR-21-31188)

Lin, Y., Y. Yang and X. Zhang. Making Invisible Visible: Data-Driven Seismic Inversion with Physics-Driven Data Augmentation. Submitted to *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*. (LA-UR-21-22294)

Lin, Y. and C. Deng. On the Robustness and Generalization of Deep Learning Driven Full Waveform Inversion. Submitted to *SIAM journal on mathematics of data science*. (LA-UR-21-31667)

Lin, Y. and X. Zhang. Spatio-Temporal Graph Convolutional Networks for Earthquake Source Characterization. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-21-20806)

Conference Papers

Lin, Y., B. E. Wohlberg and J. P. Theiler. Physics-Consistent Data-driven Seismic Inversion with Adaptive Data Augmentation. Presented at *the 34th Conference on Neural Information Processing Systems (NeurIPS)*. (Vancouver, Canada, 2020-12-06 - 2020-12-06). (LA-UR-20-27731)

Lin, Y., Q. Zeng, S. Feng and B. E. Wohlberg. 3D FullWaveform Inversion via Deep Encoder-Decoder Networks. Presented at *SEG 2021 Annual Meeting*. (denver, Colorado, United States, 2021-09-26 - 2021-09-26). (LA-UR-21-23217)

Lin, Y., Y. Yang and X. Zhang. Enhancing Data-Driven Seismic Inversion using Physics-Guided Spatiotemporal Data Augmentation. Presented at *SEG 2021 Annual Meeting*. (denver, Colorado, United States, 2021-09-26 - 2021-09-26). (LA-UR-21-23216)

Lin, Y. and B. E. Wohlberg. How Good Is Your Scientific Data Generative Model?. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*. (denver, Colorado, United States, 2020-11-15 - 2020-11-15). (LA-UR-20-27518)

Presentation Slides

Lin, Y. Demystifying Career in National Lab. Presented at *Professional Development Seminar at the School of Mathematical and Statistical Sciences, ASU*, tempe, Arizona, United States, 2020-11-16 - 2020-11-16. (LA-UR-20-29376)

Lin, Y. Subsurface Geophysical Imaging. Presented at *LANL-BEG Workshop*, Los Alamos, New Mexico, United States, 2021-04-15 - 2021-04-15. (LA-UR-21-23653)

Lin, Y. Physics-Guided Learning-Driven Computational Seismic Imaging: from Synthetic Practice to Field Applications. Presented at *AAAI Fall Symposium Series (FSS) 2021 - second Symposium on Science-Guided AI (Virtual)*, Los Alamos, New Mexico, United States, 2021-11-04 - 2021-11-06. (LA-UR-21-31071)

Lin, Y., B. E. Wohlberg, J. P. Theiler and S. Feng. Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches. . (LA-UR-21-22633)

Lin, Y., D. Coblentz, P. A. Johnson, R. J. Pawar, G. D. J. Guthrie, J. P. Theiler, B. E. Wohlberg, S. Feng and Q. Zeng. Physics-Guided Learning-Driven Computational Seismic Imaging: from Synthetic Practice to Field Applications. Presented at *Machine Learning in Solid Earth Geoscience (Online Seminar Series)*, Los Alamos, New Mexico, United States, 2021-09-10 - 2021-09-10. (LA-UR-21-28839)

Lin, Y., S. Feng, P. Jin, B. E. Wohlberg and J. D. Moulton. CycleFCN: A Physics-Informed Data-driven Seismic Waveform Inversion Method. Presented at *SEG Annual Meeting*, Houston, Texas, United States, 2020-10-12 - 2020-10-12. (LA-UR-20-28299)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. Monitoring and Forecasting CO2 Storage in the Sleipner area with Spatio-temporal CNNs. Presented at *SEG Annual Conference*, denver, Colorado, United States, 2021-09-26 - 2021-09-26. (LA-UR-21-28468)

Lin, Y., S. Feng and B. E. Wohlberg. InversionNet3D: Efficient and Scalable Learning for 3D Full Waveform Inversion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31917)

Lin, Y., Y. Yang and B. E. Wohlberg. How Good Is Your Scientific Data Generative Model?. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)*, denver, Colorado, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-27918)

Lin, Y., Y. Yang and X. Zhang. Enhancing data-driven seismic inversion using physics-guided spatiotemporal data augmentation. Presented at *SEG Annual Meeting*, denver, Colorado, United States, 2021-09-26 - 2021-09-26. (LA-UR-21-28469)

Posters

Lin, Y., C. Deng and S. Feng. Physics semantic Data Augmentation via Disentangled Representation Learning. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-32189)

Lin, Y., S. Feng, X. Zhang, B. E. Wohlberg and N. P. Symons. 4D Seismic Monitoring and Forecasting of CO2 Sequestration with Neural Networks. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31916)

Lin, Y., S. Feng and B. E. Wohlberg. Style transfer as Data Augmentation for Multiscale Data-driven Full Waveform Inversion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31915)

Lin, Y., Y. Liu and S. Feng. Mitigating data scarcity for joint physics-based and data-driven time-lapse seismic inversion. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31785)

Other

Lin, Y. OpenFWI Dataset Documentation. Dataset. (LA-UR-21-30410)

Lin, Y. Style-transfer Data Documentation. Dataset. (LA-UR-21-30948)

Lin, Y. OpenFWI Data Documentation. Dataset. (LA-UR-21-30947)

On-machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication

Wendel Brown
20210586MFR

Project Description

Precision plutonium shell machining is a key process in the flowsheet for pit manufacturing at the Plutonium Facility at Los Alamos National Laboratory (LANL). The quality of machined shells is assessed against extremely tight specifications for geometric dimensions. Fabrication of these critically important shells has historically been challenging, primarily due to plutonium deforming under dynamic cutting forces from the cutting tool. Other sources of dimensional error can be attributed to temperature fluctuations, operator setup difficulties, and mechanical issues with the machine tool. All of these error sources can be compensated for in the part program, if they can be determined while the shell is mounted on the machine. By measuring points on the surface of the shells and then compensating for dimensional errors, it is expected that a greater than 90 percent product yield can be achieved.

Publications

Presentation Slides

Brown, W. G. Mid-year Project Review on 20210586MFR "On-Machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication". . (LA-UR-21-22488)

Toward Automated Interpretation of Large, High Resolution Computed Tomography Volumes (U)

Christopher Stull
20200485MFR

Project Description

The use of Computed Tomography (CT or, in the medical field, CAT scan) as an inspection modality for weapons' components has seen a dramatic increase during the past decade, and especially during the past five years. The efficiency of CT interpretation is largely driven by staff availability and computing resources, due to the labor-dependent state-of-the-practice of staff manually examining 100s to 1000s of images. Thus far, automated interpretation of large, high resolution CT volumes, in particular, has proven difficult even with modern, commercially-available visualization software and cutting edge computing resources. Technological advances have made such large, high resolution CT volumes more readily attainable in terms of the Los Alamos Stockpile Stewardship mission, which necessitates research and development efforts to insure CT interpretation does not become a substantial bottleneck in the inspection process. The present proposal aims to address this potential shortcoming by leveraging PetaVision, a neural simulation toolbox developed at Los Alamos over the past decade, that has a proven track record of image classification on institutional class computing systems (e.g. Trinity). This effort is expected to yield a semi-automated means by which large, high resolution CT volumes may be interpreted with limited input by staff.

Technical Outcomes

The goal of this project was to implement the Los Alamos National Laboratory-developed PetaVision software to support automated interpretation of large, computed tomography data. Building on Phase 1's successes, Phase 2's efforts were focused on classified data of high mission relevance. Despite challenges imposed by COVID-19, the end result of the project provided several examples where defects were detected by way of our methodology, which in these instances, aligned with human results.

Launch Vehicle Detection and Tracking System

John Scott
20200664DI

Project Description

This proposed project is a first step to implementing a resilient architecture to address the Find-Fix-Track portion of the military's target kill chain (Find-Fix-Track-Target-Engage-Assess). The proposed system will be capable of detecting the launch of a target-of-interest, tracking the target's trajectory, and predicting its destination. This system will provide early warning of potential threats to warfighters and provide critical information for intercepting these vehicles before they reach their intended target.

Technical Outcomes

The team completed the development of a piece of Los Alamos National Laboratory software to aid in system design for a constellation of radar-equipped satellites that are meant to detect and track a vehicle moving at 50 to 100 miles of attitude. This tool addresses basic satellite design issues like number of satellites, required power and signal quality to track a vehicle with a given flight path.

Publications

Reports

Scott, J. M., N. Dallmann, J. M. Durham, W. Junor, M. Malone, R. T. Thornton, T. E. I. Tierney, B. E. Carlsten, M. P. Hoffmann and M. R. A. Zuboraj. Vehicle Tracking. Unpublished report. (LA-UR-21-31784)

Presentation Slides

Durham, J. M. and R. T. Thornton. Director's Initiative LDRD: Launch Vehicle Detection and Tracking 20200664DI. . (LA-UR-20-30319)

I. Tierney, T. E. The Challenging Plasma Environment of Hypersonic Weapons. . (LA-UR-21-24637)

Artificial Intelligence for Sensing

Aric Hagberg
20200669DI

Project Description

This project addresses national security challenges in sensing by exploring and developing modern artificial intelligence (AI) algorithms for use at sensor locations. Sensors typically have limited computing capability and are unsuitable for complicated compute-intense algorithms. New AI techniques such as deep learning, can exploit limited computing by using a combination of high performance computing for training algorithms on large existing data sets and lower-performance computing at the sensor that use the trained algorithms for analysis or prediction. The expected outcomes of this research project are identification of sensor challenges where Los Alamos has significant strategic opportunity to create advantages with AI, creation of new interdisciplinary teams and new communities of researchers connecting AI experts with engineers and sensor experts, and development of one or more technology advances using AI/Machine Learning algorithms for sensing in a Los Alamos application. National security mission applications with high potential for AI impact are: satellite and remote collection, additive manufacturing, cyber-physical security, and data analysis at scientific user facilities.

Technical Outcomes

The project developed new artificial intelligence algorithms to analyze and identify key signatures in national security mission applications of satellite and remote collection, additive manufacturing, cyber-physical security, and data analysis at scientific user facilities. The artificial intelligence algorithms developed for the specific application of additive manufacturing were used in conjunction with acoustic sensors and edge computing devices to build an in situ monitoring technology that identifies pore defects during the additive manufacturing process.

Publications

Journal Articles

Tempelman, J. R., M. K. Mudunuru, S. Karra, A. J. Wachtor, B. Ahmmed, E. B. Flynn, J. B. Forien, G. Guss, N. Calta, J. P. DePond and M. Matthews. Machine Learning to Discover Pore Formation Signatures and Predict Pore Formation in Additive Manufacturing Process. Submitted to *Additive Manufacturing*. (LA-UR-20-29189)

Presentation Slides

Karra, S. AI@Sensors progress update to LDRD. . (LA-UR-21-24324)

Oyen, D. A., C. M. Sweeney, J. L. Barber, K. M. Mertes and N. Panda. Deep Learning to Accelerate Ptychography: AI@Sensor Rapid Response. . (LA-UR-20-27401)

Reinisch, E. C., C. X. Ren, A. F. Roberts, C. J. Wilson, P. B. Eriksson and A. Ziemann. Remote sensing of polar ice: combining synthetic aperture radar and machine learning for operational navigability. Presented at *SPIE Defense +Commercial Sensing 2021*, (virtual), New Mexico, United States, 2021-04-12 - 2021-04-16. (LA-UR-21-22747)

Sweeney, C. M. Deep Learning-Assisted Image Reconstruction of Scanned Samples from X-ray Diffraction (XRD) (A.K.A. Ptychography). . (LA-UR-21-22122)

Sweeney, C. M. Towards Automated Nanoscale Imaging at Emerging X-Ray Light Sources through AI-enabled Ptychography. Presented at *Towards an Ultra-Compact X-ray Free-Electron Laser*, Virtual, California, United States, 2021-07-19 - 2021-07-20. (LA-UR-21-31411)

Quantum Algorithm Development for Optimization

Stephan Eidenbenz
20200671DI

Project Description

The quantum optimization project will develop novel and analyze existing quantum computing algorithms used for optimization problems that occur in various mission areas, such as optimum satellite or sensor placement for event detection in non-proliferation activities and process scheduling problems in high-performance computing in the stockpile stewardship mission. Quantum computing algorithms have the potential to outperform their classical counterparts significantly and thus have the potential to overcome current strategic computing limits. We aim to identify and quantify from a theoretical and experimental perspective the advantage that quantum optimization can achieve over classical-only optimization. Our approach will combine follow along two tracks: In an experimental track, where we run experiments on various Noisy Intermediate-Scale Quantum (NISQ) Devices, such as our own D-Wave quantum annealer, the International Business Machines (IBM) Quantum computer; in the theoretical track, this project will mathematically proof performance bounds of existing optimization algorithms and use these insights to develop novel provable quantum optimization algorithms.

Technical Outcomes

The quantum optimization algorithm project designed novel algorithms by expanding and redefining the Quantum Alternating Operator Ansatz (QAOA). The main results are the following: (i) design of the Grover Mixer QAOA algorithm (ii) proposal of threshold-based quantum optimization, (iii) design of a fair sampling scheme for quantum devices. Overall, these results present a significant step forward toward understanding the ability of quantum computers and Noisy Intermediate Scale Quantum (NISQ) devices to heuristically solve quantum algorithms.

Publications

Journal Articles

Aktar, S., A. Baertschi, A. Badawy and S. J. Eidenbenz. A Divide-and-Conquer Approach to Dicke State Preparation. Submitted to *IEEE Transactions on Quantum Engineering*. (LA-UR-21-31138)

Golden, J. K., A. Baertschi, D. O'Malley and S. J. Eidenbenz. QAOA-based Fair Sampling on NISQ Devices. Submitted to *ACM Transactions on Quantum Computing*. (LA-UR-21-20101)

Golden, J. K., D. O'Malley, S. J. Eidenbenz and A. Baertschi. QAOA Mixer Comparison and Experimental Quantum Advantage for Constrained Optimization Problems. Submitted to *Physical Review Letters*. (LA-UR-22-20645)

Golden, J. K., D. O'Malley, S. J. Eidenbenz and A. Baertschi. QAOA Mixer Comparison and Experimental Quantum Advantage for Constrained Optimization Problems. Submitted to *Physical Review Letters*. (LA-UR-22-20645)

Vuffray, M. D., C. J. Coffrin, Y. A. Kharkov and A. Lokhov. Programmable Quantum Annealers as Noisy Gibbs Samplers. Submitted to *Science*. (LA-UR-20-28047)

Conference Papers

Baertschi, A. and S. J. Eidenbenz. Grover Mixers for QAOA: Shifting Complexity from Mixer Design to State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Broomfield, Colorado, United States, 2020-10-12 - 2020-10-16). (LA-UR-20-23893)

Golden, J. K., A. Baertschi, D. O'Malley and S. J. Eidenbenz. Threshold-Based Quantum Optimization. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Virtual, New Mexico, United States, 2021-10-18 - 2021-10-22). (LA-UR-21-25835)

R. Pelofske, E. A., J. K. Golden, A. Baertschi, D. O\'Malley and S. J. Eidenbenz. Sampling on NISQ Devices: "Who\'s the Fairest One of All?\'". Presented at *QCE21*. (N/A - Virtual conference, New Mexico, United States, 2021-10-18 - 2021-10-22). (LA-UR-21-25803)

Presentation Slides

Baertschi, A., S. J. Eidenbenz and J. Cook. The Quantum Alternating Operator Ansatz on Maximum k-Vertex Cover. Presented at *IEEE International Conference on Quantum*

Computing and Engineering, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28067)

Baertschi, A., S. J. Eidenbenz and J. Cook. The Quantum Alternating Operator Ansatz on Maximum k-Vertex Cover. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28072)

Baertschi, A. and S. J. Eidenbenz. Grover Mixers for QAOA: Shifting Complexity from Mixer Design to State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28058)

Baertschi, A. and S. J. Eidenbenz. Grover Mixers for QAOA: Shifting Complexity from Mixer Design to State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28071)

Vuffray, M. D., A. Lokhov, C. J. Coffrin and J. A. Nelson. Programmable Quantum Annealers as Noisy Boltzmann Samplers. Presented at *D-Wave Qubits 2020*, online, New Mexico, United States, 2020-09-28 - 2020-09-29. (LA-UR-20-27111)

Posters

Baertschi, A. and S. J. Eidenbenz. Grover Mixer QAOA: Feasible State Superpositions, Convergence to Optimum, and Limitations. Presented at *24th Annual Conference on Quantum Information Processing QIP 2021*, Munich, Germany, 2021-02-01 - 2021-02-05. (LA-UR-21-20773)

Machine Learning Enhanced Modeling

Enrique Batista
20200001CR-CNL

Project Description

This project will develop tools that merge optimization theory, cutting-edge computational and algorithmic machine learning methods, with physical knowledge in the form of constraints, symmetries, and domain expertise regarding effective degrees of freedom. Our focus is to develop methodologies for automated model reduction and coarsening, learning macro-scale and atomistic models that capture relevant physics of micro-scale simulations, and algorithms for the optimization and control of power and infrastructure systems. The resulting technologies are applicable to a wide range of problems in chemistry, materials, biological systems, power grid modeling, and fluid dynamics. The research is done in interdisciplinary teams that include engineers, physicists, chemists, and mathematicians. Postdoctoral fellows conduct the research under the supervision of Laboratory staff scientists. The project will explore frontiers areas of research that are relevant to the Laboratory programs and missions. This work is also in perfect alignment with the Department of Energy (DOE) Office of Science "Artificial Intelligence (AI) for Science" initiative.

Publications

Journal Articles

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Submitted to *Numerical Linear Algebra with Applications*. (LA-UR-21-26100)

DeSantis, D. F., P. J. J. Wolfram, K. E. Bennett and B. Alexandrov. Coarse-grain cluster analysis of tensors with application to climate biome identification. 2020. *Machine Learning: Science and Technology*. **1** (4): 045020. (LA-UR-20-20548 DOI: 10.1088/2632-2153/abb676)

*Lovell, A. E., A. T. Mohan, P. Talou and M. Chertkov. Quantified uncertainties in fission yields from machine learning. *EPJ Web of Conferences*. **242**: 5003. (LA-UR-19-31677 DOI: 10.1051/epjconf/202024205003)

Lovell, A. E., A. T. Mohan and P. Talou. Quantifying Uncertainties on Fission Fragment Mass Yields with Mixture Density Networks. Submitted to *Journal of Physics G: Nuclear and Particle Physics*. (LA-UR-20-22632)

*Lovell, A. E., F. M. Nunes, M. Catacora-Rios and G. B. King. Recent advances in the quantification of uncertainties in reaction theory. 2021. *Journal of Physics G: Nuclear and Particle Physics*. **48** (1): 014001. (LA-UR-20-24349 DOI: 10.1088/1361-6471/abba72)

Lovell, A. E., P. Talou, I. Stetcu and K. J. Kelly. Anisotropy in fission fragment and prompt neutron angular distributions. *EPJ Web of Conferences*. **256**: 9. (LA-UR-19-31337 DOI: 10.1051/epjconf/202125600009)

Lovell, A. E., P. Talou, I. Stetcu and K. J. Kelly. Correlations Between Fission Fragment and Neutron Anisotropies in Neutron-Induced Fission. Submitted to *Physical Review C*. (LA-UR-20-22603)

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

Nelson, J., M. Vuffray, A. Y. Lokhov and C. C. Coffrin. Single-Qubit Fidelity Assessment of Quantum Annealing Hardware. 2021. *IEEE Transactions on Quantum Engineering*. **2**: 3102310. (LA-UR-21-23013 DOI: 10.1109/TQE.2021.3092710)

Nelson, T. R., B. T. Nebgen, A. J. White, Y. Zhang, H. Song, J. A. Bjorgaard, A. E. Sifain, B. Rodriguez-Hernandez, V. M. Freixas, S. Fernandez-Alberti, A. Roitberg, W. F. I. Malone and S. Tretiak. NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22362)

*Nunes, F. M., T. Poxon-Pearson, M. Catacora-Rios, L. Hlophe, J. Pereira, G. B. King, A. E. Lovell and G. Potel. Extracting capture from transfer reactions. 2020. *Journal of Physics: Conference Series*. **1668**: 012030. (LA-UR-19-31196 DOI: 10.1088/1742-6596/1668/1/012030)

Srinivasan, S., D. O'Malley, J. D. Hyman, S. Karra, H. S. Viswanathan and G. Srinivasan. Transient flow modeling in fractured media using graphs. Submitted to *Physical Review E*. (LA-UR-20-23560)

Srinivasan, S. and N. Panda. What is the gradient of a scalar function of a symmetric matrix ?. Submitted to *SIAM Journal on Matrix Analysis and Applications*. (LA-UR-19-31267)

. S. E. *. D. D. *. A. B. Truong, D. P., B. Alexandrov, D. P. Truong, E. Skau and D. Desantis. Boolean Matrix Factorization via Nonnegative Auxiliary Optimization. *IEEE Access*. **9: 117169-117177. (LA-UR-21-25283 DOI: 10.1109/ACCESS.2021.3107189)

Yang, H., D. P. Morton and D. Duque. Optimizing Diesel Fuel Supply Chain Operations for Hurricane Relief. Submitted to *IIE Transactions*. (LA-UR-20-23789)

Yang, H., O. Surer, D. Duque, D. P. Morton, B. Singh, S. J. Fox, R. Pasco, K. Pierce, P. Rathouz, Z. Du, M. Pignone, M. E. Escott, S. I. Adler, S. C. Johnston and L. A. Meyers. Design of COVID-19 Staged Alert Systems to Ensure Healthcare Capacity with Minimal Closures. Submitted to *Science*. (LA-UR-20-29654)

Zhou, G., B. T. Nebgen, N. E. Lubbers, W. F. I. Malone, A. M. Niklasson and S. Tretiak. GPU-Accelerated Semi-Empirical Born Oppenheimer Molecular Dynamics using PyTorch. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22394)

Zhou, G., N. E. Lubbers, K. M. Barros, B. T. Nebgen and S. Tretiak. Machine Learning with Domain Knowledge in Quantum Chemistry: Learning Dynamically Responsive Semi-Empirical Quantum Mechanics.. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-30735)

Conference Papers

Fobes, D. M., S. Claeys, F. Geth and C. J. Coffrin. PowerModelsDistribution.jl: An Open-Source Framework for Exploring Distribution Power Flow Formulations. Presented at *21st Power Systems Computation Conference*. (Porto, Portugal, 2020-06-29 - 2020-07-03). (LA-UR-19-29384)

Geth, F., C. J. Coffrin and D. M. Fobes. A Flexible Storage Model for Power Network Optimization. Presented at *1st International Workshop on Challenges and Opportunities in the Design and Operation of Energy Storage Systems*. (Melbourne, Australia, 2020-06-26 - 2020-06-26). (LA-UR-19-29733)

Turan, E. M., R. Kannan and J. Jaschke. Design of PID controllers using semi-infinite programming. Presented at *14th International Symposium on Process Systems Engineering*. (Kyoto, Japan, 2022-06-19 - 2022-06-23). (LA-UR-21-30807)

Books/Chapters

Srinivasan, S., J. D. Hyman, D. O'Malley, S. Karra, H. S. Viswanathan and G. Srinivasan. Machine Learning Techniques for Fractured Media. (LA-UR-20-22370)

Reports

Nelson, J. A., M. D. Vuffray, A. Lokhov, T. Albash and C. J. Coffrin. High-quality Thermal Gibbs Sampling with Quantum Annealing Hardware. Unpublished report. (LA-UR-21-28692)

Rupe, A. T., V. V. Vesselinov, B. T. Nadiga, D. F. DeSantis and M. Anghel. Transfer Operator Framework for Earth System Predictability and Water Cycle Extremes. Unpublished report. (LA-UR-21-22681)

Suau, A., J. A. Nelson, M. D. Vuffray, A. Lokhov, L. Cincio and C. J. Coffrin. Single-Qubit Cross Platform Comparison of Quantum Computing Hardware. Unpublished report. (LA-UR-21-28409)

Presentation Slides

Kazi, S. R., M. Thombre and L. T. Biegler. Hybrid Strategy for solving MPECs. Presented at *AIChE Annual Meeting*, Boston, Massachusetts, United States, 2021-11-07 - 2021-11-11. (LA-UR-21-30789)

Lovell, A. E. Uncertainty Quantification for Reaction Theory. . (LA-UR-20-23038)

Lovell, A. E., A. T. Mohan, P. Talou and M. Chertkov. Predicting Fission Yields with Mixture Density Networks. Presented at *Microscopic Approaches to Nuclear Structure and Reactions*, Livermore, California, United States, 2019-11-12 - 2019-11-12. (LA-UR-19-31199)

Lovell, A. E., A. T. Mohan and P. Talou. Probabilistic Machine Learning for Uncertainty Quantification. Presented at *Machine Learning for Nuclear Data*, Online, New Mexico, United States, 2020-12-08 - 2020-12-08. (LA-UR-20-29925)

Rupe, A. T. Ergodic Theory and Dynamical Process Modeling. . (LA-UR-21-20546)

Rupe, A. T. Learning Implicit Models of Complex Dynamical Systems From Partial Observations. . (LA-UR-21-26946)

Rupe, A. T. The Search For Thermodynamic Principles of Organization. . (LA-UR-21-27304)

Rupe, A. T., K. Kashinath and J. P. Crutchfield. Discovering Emergent Organization in Complex Spatiotemporal Systems. Presented at *AGU*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31934)

Teti, M. A. CNNs With a Neuromorphic Sparse Coding Frontend are More Robust to Adversarial Attacks. Presented at *Naval Applications of Machine Learning (NAML)*, Virtual, California, United States, 2022-03-22 - 2022-03-24. (LA-UR-22-21808)

Teti, M. A. CNNs With a Neuromorphic Sparse Coding Frontend are More Robust to Adversarial Attacks. Presented at *Naval Applications of Machine Learning (NAML)*, Virtual, California, United States, 2022-03-22 - 2022-03-24. (LA-UR-22-22116)

Weisser, T. Recover Functional Relations from Moment Information. Presented at *Arizona Days*, Los Alamos, New

Mexico, United States, 2020-05-18 - 2020-05-18. (LA-UR-20-23852)

Yang, H. and H. Nagarajan. Distribution Network Optimization under Stochastic Disruptions. Presented at *INFORMS Annual Meeting 2020*, Online, New Mexico, United States, 2020-11-07 - 2020-11-13. (LA-UR-20-28337)

Yang, H. and H. Nagarajan. Distribution Network Optimization Under Stochastic Disruptions. Presented at *INFORMS Annual Meeting 2020*, Online, New Mexico, United States, 2020-11-07 - 2020-11-13. (LA-UR-20-28580)

Zhou, G., N. E. Lubbers, K. M. Barros, B. T. Nebgen and S. Tretiak. Machine Learning with Domain Knowledge in Quantum Chemistry. Presented at *Telluride Workshop "Machine Learning and Informatics for Chemistry and Materials"*, Telluride, Colorado, United States, 2021-09-27 - 2021-10-01. (LA-UR-21-29365)

Posters

Rupe, A. T., V. V. Vesselinov and J. P. Crutchfield. Connecting Physics-Based and Data-Driven Approaches for Predicting Earth Systems from Partial Observations. Presented at *AGU*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31850)

Information Science and Technology Institute (ISTI): Foundational Research in Information Science and Technology

James Ahrens
20210529CR-IST

Project Description

This Information, Science and Technology (IS&T) project addresses national security challenges in the Department of Energy/National Nuclear Security Administration Defense Program mission space. Maintaining the stockpile requires the simulation of materials under extreme conditions. Goals of this proposal include supporting a collection of IS&T projects that explore using either artificial intelligence, quantum computing or configurable hardware to create faster, higher-fidelity simulations. Another goal focuses on understanding and validating these simulations using advanced data science methods. This proposal also contributes to the DOE NNSA Nuclear Nonproliferation mission. This mission is to prevent actors from developing nuclear weapons or acquiring weapons-usable nuclear or radiological materials, equipment, technology, and expertise. Achieving this mission requires use of data and methods to detect these activities. To be successful, a final goal is to develop methods that ensure our data and methods are of the highest integrity and have not been manipulated in any way. The expected result of this proposal is to create a collection of high-risk, high-rewards IS&T projects that addresses Los Alamos National Laboratory mission needs. These projects will support workforce development by funding students, post-doctoral scholars and staff.

Publications

Journal Articles

Karra, S., B. Ahmmed and M. Mudunuru. AdjointNet: Constraining machine learning models with physics-based codes. Submitted to *Journal of Computational Physics*. (LA-UR-21-28763)

Yoon, B., C. C. Chang, G. Kenyon, N. T. T. Nguyen-Fotiadis and E. Rrapaj. Prediction and compression of lattice QCD data using machine learning algorithms on quantum annealer. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-31665)

Presentation Slides

Ahrens, J. P. Information Science and Technology Institute Rapid Response R&D and Institutional Program Development programs – Round 1 & 2. . (LA-UR-21-21664)

Brady, P. T., D. Livescu and N. Sharan. AI Enhanced Discretizations for High-Fidelity Physics Simulations. . (LA-UR-21-29077)

Carpenter, M. H., E. S. Teti and S. Salazar Escobedo. Machine Learning for Hyperspectral X-ray Imaging Analysis. . (LA-UR-21-28927)

Castorena, J. E. Boosting Deep Semi-Supervised Learning with Multi-view Redundant Information. . (LA-UR-21-28998)

DeStefano, Z. L. Distributed and Verifiable Uncertainty Quantification Using Zero Knowledge Proofs. . (LA-UR-21-26797)

DeStefano, Z. L. Distributed and Verifiable Uncertainty Quantification Via Zero Knowledge Proofs. . (LA-UR-21-27618)

Dixon, M. J., Z. L. DeStefano and D. A. Barrack. Private and Verifiable Model Evaluation using Secure Multiparty Computation and Zero-knowledge Proofs. Presented at *ISTI Rapid Response Review*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-28963)

Moore, E. A., J. B. Nakhleh, E. C. W. Drobina and S. Hazarika. Explanations as Defense: Detecting Adversarial Inputs to Machine Learning Models. . (LA-UR-21-28972)

Rego, J. R., E. Kim and G. Kenyon. Biologically Inspired Robust Perception Approximating Sparse Coding. . (LA-UR-21-29039)

Solander, K. C., C. J. Talsma and V. V. Vesselinov. Wildfire reburns and diminishing returns of existing forest management policies. Presented at *ISTI Program (LANL) Year End Review*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-28987)

Tang, L. Performance Modeling of Scientific Codes on Machine Learning Accelerators. . (LA-UR-21-28949)

Teti, E. S. Robotic Olfaction, Human Color Perception, and X-ray Emission Spectroscopy: Victims of "Unfortunate Data". . (LA-UR-21-30342)

Wilinski, M. J. Statistical inference for network dynamics. Presented at *ISTI Year-End Review*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-29024)

Wilinski, M. J. Learning of the full dynamic system state matrix from partial PMU observations. . (LA-UR-22-21926)

Yoon, B. Unbiased Reconstruction of Lossy-compressed Statistical Data. Presented at *ISTI Year-End Review*, Los Alamos, New Mexico, United States, 2021-09-13 - 2021-09-13. (LA-UR-21-28904)

Yoon, B. Machine Learning Prediction and Compression of Lattice QCD Observables. Presented at *Machine Learning for High Energy Physics, on and off the Lattice*, Trento, Italy, 2021-09-27 - 2021-09-27. (LA-UR-21-29432)

Materials for the Future

Proximity Effects at Meso-, Nano-, and Atomic Scales: A new Path to Quantum Functionalities

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Project Description

Devices based on quantum phenomena are rapidly emerging as enablers for new classes of sensors and detectors as well as for quantum information technologies. Operation of almost all of these devices relies on the ability to generate, manipulate, and detect truly quantum degrees of freedom (DOF), such as spin-up or spin-down state of electrons, or the so-called "valley pseudospin" DOF that is accessible in atomically-thin 2-Dimensional semiconductors. Here, we propose an original approach to significantly broaden the functionality of atomically-thin semiconductors by exploiting novel proximity effects – the phenomenon by which a thin material acquires magnetic properties of an adjacent material via quantum-mechanical interactions. A key innovation of our proposed work is to localize proximity effects to meso-, nano- and atomic scales, rather than inducing effects globally. This will (1) enable an unprecedented ability to manipulate valley pseudospin transport, and (2) open new avenues for transfer of information between valley pseudospin and photon quantum states. With these two aims, we expect our project to bring transformational breakthroughs in the emerging field of "valleytronics", where valley pseudospin is exploited to store and carry information, as well as photonic quantum technologies promising eavesdropping proof communications.

Publications

Journal Articles

Bittner, E. R., H. Li, A. Piryatinski, A. R. S. Kanda and C. Silva. Probing exciton/exciton interactions with entangled photons: theory. Submitted to *Journal of Chemical Physics*. (LA-UR-20-20751)

*Chen, A. and Q. Jia. A pathway to desired functionalities in vertically aligned nanocomposites and related architectures. 2021. *MRS Bulletin*. **46** (2): 115-122. (LA-UR-21-21607 DOI: 10.1557/s43577-021-00032-4)

*Chernyak, V. Y., N. A. Sinitsyn and C. Sun. Dynamic spin localization and \xce\xb3-magnets. 2019. *Physical Review B*. **100** (22): 224304. (LA-UR-19-24184 DOI: 10.1103/PhysRevB.100.224304)

*Choudhary, K., K. F. Garrity, A. C. E. Reid, B. DeCost, A. J. Biacchi, A. R. H. Walker, Z. Trautt, J. Hattrick-Simpers, G. Kusne, A. Centrone, A. Davydov, J. Jiang, R. Pachter, G. Cheon, E. Reed, A. Agrawal, X. Qian, V. Sharma, H. Zhuang, S. V. Kalinin, B. G. Sumpter, G. Pilania, P. Acar, S. Mandal, K. Haule, D. Vanderbilt, K. Rabe and F. Tavazza. The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. 2020. *npj Computational Materials*. **6** (1): 173. (LA-UR-20-25348 DOI: 10.1038/s41524-020-00440-1)

Choudhary, K., K. F. Garrity, G. Pilania and F. Tavazza. Efficient Computational Design of 2D van der Waals Heterostructures: Band-Alignment, Lattice-Mismatch, Web-app Generation and Machine-learning. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-20-22997)

Crooker, S. A., M. Goryca, J. Li, S. Tongay, K. Yumigeta and H. Li. Carrier-density-dependent valley relaxation in a monolayer semiconductor and the role of substrate-induced disorder. Submitted to *Physical Review Applied*. (LA-UR-21-20744)

Crooker, S. A., M. M. Goryca, J. Li, J. Choi and X. Xu. Many-Body Exciton and Intervalley Correlations in Heavily Electron-Doped WSe2 Monolayers. 2022. *Nano Letters*. **22** (1): 426-432. (LA-UR-21-31300 DOI: 10.1021/acs.nanolett.1c04217)

*Enriquez, E. M., Q. Li, P. R. Bowlan, P. Lu, B. Zhang, L. Li, H. Wang, A. J. Taylor, D. A. Yarotski, R. P. Prasankumar, S. V. Kalinin, Q. Jia and A. Chen. Induced ferroelectric phases in SrTiO by a nanocomposite approach. 2020. *Nanoscale*. **12** (35): 18193-18199. (LA-UR-20-24150 DOI: 10.1039/D0NR03460F)

Grefe, S. E., Q. Si, H. Lai and S. Paschen. Extreme response of Weyl-Kondo semimetal to Zeeman coupling. Submitted to *Physical Review Letters*. (LA-UR-20-30516)

Hartman, S. T. and G. Pilania. Strong Zeeman Splitting in Orbital-Hybridized Valleytronic Interfaces. Submitted to *Journal of Materials Science*. (LA-UR-21-29703)

Kang, K. T., B. Zhang, Y. Sharma, B. Paudel, H. Wang, P. Dowden and A. Chen. Substrate oxygen sponge effect: a parameter for epitaxial manganite thin film growth. Submitted to *Applied Physics Letters*. (LA-UR-20-28258)

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

*Koraltan, S., S. Slanovc, F. Bruckner, C. Nisoli, V. A. Chumak, V. O. Dobrovolskiy, C. Albert and S. Dieter. Tension-free Dirac strings and steered magnetic charges in 3D artificial spin ice. 2021. *npj Computational Materials*. **7** (1): 125. (LA-UR-21-21222 DOI: 10.1038/s41524-021-00593-7)

*Lane, C. Interlayer coupling induced quasiparticles. 2020. *Physical Review B*. **101** (23): 235138. (LA-UR-20-23062 DOI: 10.1103/PhysRevB.101.235138)

Lane, C. A. and J. Zhu. Thickness dependence of electronic structure and optical properties of a correlated van der Waals antiferromagnet NiPS3 thin film. Submitted to *Physical Review B*. (LA-UR-20-22026)

*Li, J., S. A. Crooker, M. M. Goryca, A. V. Stier, N. Wilson and X. Xu. Spontaneous Valley Polarization of Interacting Carriers in a Monolayer Semiconductor. 2020. *Physical Review Letters*. **125** (14): 147602. (LA-UR-20-25746 DOI: 10.1103/PhysRevLett.125.147602)

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

Malla, R. K., V. Y. Chernyak, C. Sun and N. Sinitsyn. Coherent reaction between molecular and atomic Bose-Einstain condensates: integrable model. Submitted to *Physical Review Letters*. (LA-UR-21-32402)

Malla, R. K., V. Y. Chernyak and N. Sinitsyn. Nonadiabatic transitions in Landau-Zener grids: integrability and semiclassical theory. Submitted to *Physical Review B*. (LA-UR-21-20136)

*Nisoli, C. The concept of spin ice graphs and a field theory for their charges. 2020. *AIP Advances*. **10** (11): 115102. (LA-UR-20-24780 DOI: 10.1063/5.0010079)

*Nisoli, C. Equilibrium field theory of magnetic monopoles in degenerate square spin ice: Correlations, entropic interactions, and charge screening regimes. 2020. *Physical Review B*. **102** (22): 220401. (LA-UR-20-24779 DOI: 10.1103/PhysRevB.102.220401)

Nisoli, C. Gauge-free duality in pure square spin ice: Topological currents and monopoles. 2021. *AIP Advances*. **11** (10): 105313. (LA-UR-21-28824 DOI: 10.1063/5.0070545)

*K. K. T. *. S. Y. *. N. H. *. Y. D. *. C. A. Paudel, B. *., B. Paudel, K. T. Kang, Y. Sharma, A. Chen and D. Yarotski. Symmetry mismatch controlled ferroelastic domain ordering and the functional properties of manganite films on cubic miscut substrates. 2021. *Physical Chemistry Chemical Physics*. **23** (31): 16623-16628. (LA-UR-21-29518 DOI: 10.1039/D1CP01957K)

Paudel, B., Y. Sharma, B. K. Derby, G. Pilania, M. M. Schneider, A. C. Jones, H. Nakotte, M. T. Pettes and A. Chen. Effect of lattice strain on magnetism in epitaxial YCrO3 films. 2022. *Materials Research Letters*. **10** (1): 29-35. (LA-UR-21-30206 DOI: 10.1080/21663831.2021.2010822)

Shi, Y., C. Nisoli and G. W. Chern. Icy, Glassy, and Solid Phases via Quenched Disorder in Shakti Spin Ice. Submitted to *Applied Physics Letters*. (LA-UR-21-21120)

Sinitsyn, N., A. Fisher, I. Kleinjoharnn and F. B. Anders. Cross-correlation spectra in interacting quantum dot systems. Submitted to *Physical Review B*. (LA-UR-21-28148)

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

Wang, B., S. Yang, Y. Wang, Y. H. Kim, H. Htoon, S. K. Doorn, B. J. Foran, D. R. Baker, G. T. Forcehrio and S. B. Cronin. Formation of Brightly Luminescent MoS2 Nanoislands from Multilayer Flakes via Plasma Treatment and Laser Exposure. Submitted to *ACS Omega*. (LA-UR-20-28248)

Wei, X., H. Hui, C. Zhao, C. Deng, M. Han, Z. Yu, A. Sheng, P. Roy, A. Chen, J. Lin, D. F. Watson, Y. Sun, T. Thomay, S. Yang, Q. Jia, S. Zhang and H. Zeng. Realization of BaZrS3 chalcogenide perovskite thin films for optoelectronics. Submitted to *Nano Energy*. (LA-UR-20-24151)

*Yan, B., V. Y. Chernyak, W. H. Zurek and N. A. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. 2021. *Physical Review Letters*. **126** (7): 070602. (LA-UR-20-26742 DOI: 10.1103/PhysRevLett.126.070602)

P. M. T. *. Z. Y. *. H. H. Zhao, H. *., H. Zhao, M. T. Pettes, Y. Zheng and H. Htoon. Site-controlled telecom-wavelength single-photon emitters in atomically-thin MoTe2. 2021. *Nature Communications*. **12** (1): 6753. (LA-UR-21-23958 DOI: 10.1038/s41467-021-27033-w)

Zheng, Y., Y. H. Kim, A. C. Jones, G. Olinger, E. R. Bittner, S. M. Bachilo, S. K. Doorn, R. B. Weisman, A. Piryatinski and H. Htoon. Quantum Light Emission from Coupled Defect States in DNA-Functionalized Carbon Nanotubes. Submitted to *ACS Nano*. (LA-UR-21-24662)

Zhu, J., G. Dhakal, M. M. Hosen, A. Ghosh, C. A. Lane, K. Gornica, M. J. Winiarski, K. Dimitri, F. Kabir, C. Sims, S. Regmi, W. D. Neff, D. Kaczorowski, T. Klimczuk and M. Neupane. Observation of topological surface state in a superconducting material. Submitted to *Physical Review Letters*. (LA-UR-19-31397)

Books/Chapters

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

Presentation Slides

Alcantara, A. R., C. A. Lane, R. M. Tutchton and J. T. Haraldsen. Thickness dependence of the electronic and magnetic properties of a correlated Van der Waals magnet, CrPS4. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-19. (LA-UR-22-21903)

Chen, A. Correlation among strain, defect, interface and functional properties in oxide nanocomposites. Presented at *CINT user meeting*, los alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27407)

Chen, A. Roles of Defects and Interface in Ferroelectric Resistive Switching. Presented at *lectronic Materials and Applications 2022*, Orlando, Florida, United States, 2022-01-19 - 2022-01-19. (LA-UR-22-20424)

Grefe, S. E., H. Lai, S. Paschen and Q. Si. Extreme response of Weyl-Kondo semimetal to Zeeman coupling. Presented at *2021 American Physical Society March Meeting (Virtual/Online)*, Virtual/Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22720)

Grefe, S. E., R. P. Prasankumar, Q. Si and J. Zhu. High harmonic generation in Weyl-Kondo semimetals. Presented at *2021 American Physical Society March Meeting (Virtual/Online)*, Online/Virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22719)

Hartman, S. T. and G. Pilania. Factors Influencing Valley Splitting in 2D Heterointerfaces. Presented at *MRS Fall Meeting*, Virtual, Hawaii, United States, 2021-12-06 - 2021-12-08. (LA-UR-21-31577)

Lane, C. A. Many-Body Electron Dynamics with Interlayer Coupling. Presented at *QUANTUM MATERIALS WORKSHOP: INVESTIGATING THE INTERLAYER COUPLING AND INTERFACE IN 2D STRUCTURES*, Boston, Massachusetts, United States, 2020-01-07 - 2020-01-07. (LA-UR-20-20141)

Lane, C. A. and J. Zhu. Thickness Dependence of Electronic Structure and Optical Properties of a Correlated van der Waals Antiferromagnet: NiPS3. Presented at *CINT Annual Meeting 2021*, Los Alamos, New Mexico, United States, 2021-09-21 - 2021-09-23. (LA-UR-21-29274)

Pilania, G. Annual Report Highlight Slides for w20_MatDesign. . (LA-UR-21-23502)

Tutchton, R. M. and C. A. Lane. Summer Project Ideas. Presented at *Student Meeting*, Los Alamos, New Mexico, United States, 2021-05-06 - 2021-05-06. (LA-UR-21-24391)

Posters

Alcantara, A. R., C. A. Lane and R. M. Tutchton. Beyond GGA+U: SCAN meta-GGA on 2D Van der Waals magnet CrPS4. Presented at *UNF graduate student symposium*, Jacksonville, Florida, United States, 2021-10-21 - 2021-10-21. (LA-UR-21-30325)

Lane, C. A. and J. Zhu. Proximity Effects in Two-Dimensional Transition-Metal Dichalcogenide Materials for Quantum Information Science. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21954)

Lane, C. A. and J. Zhu. Thickness Dependence of Electronic Structure and Optical Properties of a Correlated van der Waals Antiferromagnet: NiPS3. Presented at *The 2021 CINT Annual Meeting*, Los Alamos, New Mexico, United States, 2021-09-21 - 2021-09-23. (LA-UR-21-29147)

Zhu, J., A. Ghosh and S. Lin. Data-driven study of magnetic interactions of transition-metal based 2D materials. Presented at *2020 APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-19-30770)

Control Of Microstructural Instabilities in Composites (COMIC): A Pathway to Realizing Damage Resistant Metals

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Project Description

This project will deliver an integrated multi-scale modeling framework for the prediction of the relationship between metallic microstructure, loading conditions and ductility. In simpler terms, it will provide the ground-breaking tools needed to predict when failure will occur in metallic materials. This will be enabled by processing and characterizing hitherto not explored/exploited nanometallic composites such as to allow for the validation of a generalized failure model. As a metric of success, this model will be used to design composites with superior ductility. In the long term, Control Of Microstructural Instabilities in Composites (COMIC) will pave the way towards modeling and designing more resilient metals processed through conventional or advanced manufacturing techniques. This can have Los Alamos-centered impact within potential transition to the National Nuclear Security Administration's advanced manufacturing development program and national missions in energy security by providing pathways to realize light-weighting.

Publications

Journal Articles

Bamney, d., R. Royce, L. Capolungo and D. E. Spearot. Disclination-dislocation based model for grain boundary stress field evolution due to slip transmission history and influence on subsequent dislocation transmission. Submitted to *Journal of the Mechanics and Physics of Solids*. (LA-UR-21-31117)

*L. R. A. Berbenni, S. *. and R. A. Lebensohn. A numerical study of reversible plasticity using continuum dislocation mechanics. 2021. *Comptes Rendus. Physique*. **22** (S3): 295-312. (LA-UR-21-32396 DOI: 10.5802/crphys.54)

Carpenter, J. S., D. J. Savage, C. Miller, R. J. Mccabe, S. Zheng, D. R. Coughlin and S. C. Vogel. Accumulative Roll Bonding of Alloy 2205 Duplex Steel and the Accompanying Impacts on Microstructure, Texture, and Mechanical Properties. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-22-22594)

Chakraborty, A., A. Hunter and L. Capolungo. Effect of microstructure, layer thickness, and interface behavior on the plasticity of accumulative roll bonded nano-metallic laminates using dislocation dynamics simulations. Submitted to *Journal of Materials Research*. (LA-UR-20-30289)

Chen, J. and S. J. Fensin. Effect of Local Structure and Stoichiometry on the Dynamic Behavior of Bi-metal interfaces. Submitted to *Journal of Applied Physics*. (LA-UR-21-22436)

Christodoulou, P., R. A. Lebensohn and I. Beyerlein. FFT-based study of the interplay between lower-order and higher-order energetic strain-gradient effects in polycrystal plasticity. Submitted to *Journal of the Mechanics and Physics of Solids*. (LA-UR-21-32270)

Dong, S., X. Liu and C. Zhou. Atomistic modeling of plastic deformation in B2-FeAl/Al nanolayered composites. Submitted to *International Journal of Plasticity*. (LA-UR-21-21266)

Genee, J., N. Gey, F. Bonnet, R. A. Lebensohn and S. Berbenni. Experimental and numerical investigation of key microstructural features influencing the localization of plastic deformation in Fe-TiB2 metal matrix composite. Submitted to *Journal of Materials Science*. (LA-UR-22-20642)

Liu, X., L. Capolungo and A. Hunter. Screw dislocations impingement and slip transfer at fcc-bcc semicoherent interfaces. Submitted to *Scripta Materialia*. (LA-UR-21-20512)

Ma, X., B. Gwalani, J. Tao, M. Efe, M. Olszta, M. Song, S. Yadav, A. Yu, T. J. Nizolek, J. S. Carpenter, B. Zhou, A. Devaraj, S. Mathaudhu and A. Rohatgi. Shear strain gradient in Cu/Nb nanolaminates: strain accommodation and chemical mixing. Submitted to *Acta Materialia*. (LA-UR-21-31147)

McCabe, R. J., T. J. Nizolek, N. Li, Y. Zhang, D. R. Coughlin, C. Miller and J. S. Carpenter. Evolution of microstructures and properties leading to layer instabilities during accumulative roll bonding of Fe Cu, Fe Ag, and Fe Al. 2021.

Materials & Design. **212**: 110204. (LA-UR-21-30621 DOI: 10.1016/j.matdes.2021.110204)

Mccabe, R. J., T. J. Nizolek, N. Li, Y. Zhang, D. R. Coughlin, C. Miller and J. S. Carpenter. Evolution of Microstructures and Properties Leading to Layer Instabilities during Accumulative Roll Bonding of Fe-Cu, Fe-Ag, and Fe-Al. Submitted to *Materials & Design*. (LA-UR-21-28391)

*Nizolek, T. J., T. M. Pollock and R. M. McMeeking. Kink Band and Shear Band Localization in Anisotropic Perfectly Plastic Solids. 2020. *Journal of the Mechanics and Physics of Solids*. 104183. (LA-UR-20-25448 DOI: 10.1016/j.jmps.2020.104183)

K. B. *. B. M. *. N. T. *. W. Y. *. K. M. *. M. N. *. A. O. Radhakrishnan, M. *., T. J. Nizolek and Y. Q. Wang. Layer dissolution in accumulative roll bonded bulk Zr/Nb multilayers under heavy-ion irradiation. 2021. *Journal of Nuclear Materials*. **557**: 153315. (LA-UR-21-24055 DOI: 10.1016/j.jnucmat.2021.153315)

*Zecevic, M., K. C. Bennett, D. J. Luscher and R. A. Lebensohn. New self-consistent homogenization for thermo-elastic polycrystals with imperfect interfaces. 2021. *Mechanics of Materials*. **155**: 103651. (LA-UR-20-24726 DOI: 10.1016/j.mechmat.2020.103651)

Zecevic, M., R. A. Lebensohn and L. Capolungo. New large-strain FFT-based formulation and its application to model strain localization in nano-metallic laminates and other strongly anisotropic crystalline materials. 2022. *Mechanics of Materials*. **166**: 104208. (LA-UR-21-29080 DOI: 10.1016/j.mechmat.2021.104208)

Zecevic, M. and R. A. Lebensohn. Approximation of periodic Green's operator in real space using numerical integration and its use in fast Fourier transform-based micromechanical models. 2021. *International Journal for Numerical Methods in Engineering*. **122** (24): 7536-7552. (LA-UR-21-23581 DOI: 10.1002/nme.6841)

Zhang, Y., N. Li, M. M. Schneider, T. J. Nizolek, L. Capolungo and R. J. Mccabe. Kink mechanism in Cu/Nb nanolaminates explored by in situ pillar compression. Submitted to *Acta Materialia*. (LA-UR-22-20465)

Presentation Slides

Adams, C. L. Fast Fourier transform (FFT)-based modelling of microstructural effects in additively manufactured (AM) metals. Presented at *2021 Lightning Talk Series*, Los Alamos, New Mexico, United States, 2021-07-27 - 2021-07-27. (LA-UR-21-27312)

Raveendranath Bamney, D., L. Capolungo and D. E. Spearot. Model for Grain Boundary Stress Field Evolution due to Dislocation-grain Boundary Interactions and Influence on Subsequent Slip Transmission. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-03-03. (LA-UR-22-21459)

Carpenter, J. S., D. R. Coughlin, R. J. Mccabe, C. Miller, T. J. Nizolek, C. M. J. Osborn and M. M. Schneider. Probing Differences in Processing and Texture in FCC/BCC Nanolaminates Fabricated via Accumulative Roll Bonding. Presented at *MS&T 2020*, Pittsburgh, Pennsylvania, United States, 2020-11-02 - 2020-11-02. (LA-UR-20-28102)

Chakraborty, A., A. Hunter and L. Capolungo. Capturing kinetics of FR sources using DD simulations. . (LA-UR-21-20738)

Chakraborty, A., A. Hunter and L. Capolungo. Capturing kinetics of FR sources using DD simulations. . (LA-UR-21-24423)

Chakraborty, A., A. Hunter and L. Capolungo. Capturing kinetics of FR sources using DD simulations. . (LA-UR-21-25410)

Chakraborty, A., A. Hunter and L. Capolungo. Capturing kinetics of FR sources using DD simulations. . (LA-UR-21-25437)

Chakraborty, A., A. Hunter and L. Capolungo. Modeling slip transmission across interface using dislocation dynamics simulations. Presented at *MS&T 2021*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-21. (LA-UR-21-30081)

Chakraborty, A., M. Zecevic, X. Liu, A. Hunter, R. A. Lebensohn and L. Capolungo. Understanding plasticity in nano-metallic laminates using dislocation dynamics simulations. . (LA-UR-21-21588)

Cocke, C. K., A. D. Rollett, R. A. Lebensohn and A. D. Spear. The AFRL AM Modeling Challenge: Predicting Micromechanical Fields in AM IN625 Using an FFT-based Method with Direct Input from a 3D Microstructural Image. Presented at *5th International Congress on 3D Materials Science*, Washington, District Of Columbia, United States, 2021-06-29 - 2021-07-02. (LA-UR-21-25826)

Lebensohn, R. A. Brief Overview of Polycrystal Plasticity Models. . (LA-UR-21-28799)

Mccabe, R. J., M. Zecevic, T. J. Nizolek, N. Li, M. M. Schneider, C. Miller, C. M. J. Osborn, D. R. Coughlin, R. A. Lebensohn and J. S. Carpenter. Texture evolution of individual layers during accumulative roll bonding of Fe/fcc metallic laminates. Presented at *MS&T20 Virtual*, Los Alamos, New Mexico, United States, 2020-11-02 - 2020-11-06. (LA-UR-20-28399)

Mccabe, R. J., M. Zecevic, Y. Zhang, N. Li, J. G. Gigax, T. J. Nizolek and J. S. Carpenter. Layer dependent plasticity in accumulative roll bonded FCC/BCC metallic laminates. Presented at *TMS 2021Annual Meeting & Exhibition*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21826)

Nizolek, T. J., D. R. Coughlin, C. Miller, Y. Zhang, N. Li, R. J. Mccabe, C. M. J. Osborn and J. S. Carpenter. Evolution of Mechanical Properties and Microstructure in Accumulative Roll Bonded FCC/BCC Metallic Composites. Presented at *TMS 2021 (virtual conference)*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-21746)

Schneider, M. M. Recent Advancements in Tools and Techniques for Materials Characterization in the EML. . (LA-UR-21-29078)

Zecevic, M., R. A. Lebensohn, K. Bennett and D. J. Luscher. Analytical and computational homogenization of heterogeneous microstructures with imperfect interfaces. Presented at *14th World Congress in Computational Mechanics*, Paris, France, 2021-01-11 - 2021-01-15. (LA-UR-20-29723)

Zecevic, M., R. A. Lebensohn, T. J. Nizolek, R. J. Mccabe and L. Capolungo. FFT-based modeling of strain localization in nano-metallic laminates. Presented at *TMS 2021 (virtual conference)*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21750)

Zhang, Y., N. Li, M. M. Schneider, T. J. Nizolek, R. J. Mccabe, M. Zecevic, J. S. Carpenter and L. Capolungo. Kinking in nanolaminates during in situ pillar compression. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-03-03. (LA-UR-22-21561)

Zhang, Y., N. Li, M. M. Schneider, T. J. Nizolek, R. J. Mccabe and L. Capolungo. Kinking in Cu/Nb nanolaminates during in situ pillar compression. Presented at *MS&T21 Technical Meeting and Exhibition*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-21. (LA-UR-21-29887)

Zhang, Y., Q. Li, M. Gong, T. Niu, S. Xue, J. Wang, H. Wang, X. Zhang and N. A. Richter. Deformation behavior and phase transformation of nanotwinned Al/Ti multilayers. Presented at *TMS 2021 Virtual Annual Meeting*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21787)

Quantum Photonics with Semiconductor Nanocrystals

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Project Description

The goal of this project is to exploit the unmatched flexibility of colloidal nanocrystals (NCs) for demonstrating atomic-like single-photon emitters (SPEs) with long-lived optical coherence that is preserved at elevated temperatures. In particular, this project aims to exploit a size-controlled NC band gap for realizing high-fidelity sources of quantum light with an arbitrary wavelength tunable across both visible and NIR spectral ranges. A further objective is to implement integrated NC-photonic circuits using which we will be able to excite a selected NC (or a NC group) and then readout desired information (spectral, temporal, or statistical). This will demonstrate the 'integrability' and scalability of the NC-SPE approach and, in addition, will provide a powerful capability for systematic studies of the effects of controlled photonic environment on SPE-related NC properties. The realization of high-quality NC-based SPEs will lead to a transformational impact in quantum information science (QIS) by addressing the important current challenge of "overcoming the tyranny of low temperature". The availability of highly flexible, colloidal SPEs will facilitate real-life implementations of QIS technologies especially in areas of metrology, sensing, and imaging.

Publications

Journal Articles

Bian, M., L. Zhu, X. Wang, J. Choi, S. A. Crooker, J. Lin and H. Zeng. Dative epitaxy of monocrystalline covalent-van der Waals moir\xc3\xa9 supercrystal. Submitted to *Nano Letters*. (LA-UR-22-21038)

*Fedin, I., M. Goryca, D. Liu, S. Tretiak, V. I. Klimov and S. A. Crooker. Enhanced Emission from Bright Excitons in Asymmetrically Strained Colloidal CdSe/Cd Zn Se Quantum Dots. 2021. *ACS Nano*. **15** (9): 14444-14452. (LA-UR-21-23484 DOI: 10.1021/acsnano.1c03864)

*Jung, H., N. Ahn and V. I. Klimov. Prospects and challenges of colloidal quantum dot laser diodes. 2021. *Nature Photonics*. **15** (9): 643-655. (LA-UR-21-22207 DOI: 10.1038/s41566-021-00827-6)

Klimov, V. I. Semiconductor quantum dots: Technological progress and future challenges. Submitted to *Science*. (LA-UR-20-25113)

Klimov, V. I. Highly Versatile Near-Infrared Emitters Based on an Atomically-Defined HgS Interlayer Embedded into a CdSe/CdS Quantum Dot. Submitted to *Nature Nanotechnology*. (LA-UR-20-28236)

Klimov, V. I. Colloidal Quantum Dot Lasers. Submitted to *Nature Reviews Materials*. (LA-UR-20-28237)

Klimov, V. I. Exploiting Functional Impurities for Fast and Efficient Incorporation of Manganese into Quantum Dots. Submitted to *Journal of the American Chemical Society*. (LA-UR-20-28235)

Li, J., S. A. Crooker, M. M. Goryca, A. V. Stier, N. Wilson and X. Xu. Spontaneous valley polarization of interacting carriers in a monolayer semiconductor. Submitted to *Physical Review Letters*. (LA-UR-20-25746)

Tretiak, S., M. Bhati, S. A. Ivanov and D. Ghosh. Nature of Electronic Excitations in Non-stoichiometric Quantum Dots. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-27876)

*Yun, H. J., J. Lim, J. Roh, D. C. J. Neo, M. Law and V. I. Klimov. Solution-processable integrated CMOS circuits based on colloidal CuInSe2 quantum dots. 2020. *Nature Communications*. **11** (1): 5280. (LA-UR-20-25114 DOI: 10.1038/s41467-020-18932-5)

Reports

Robinson, Z. L. Electronic and Optical Properties of Quantum Dots: Metal-Insulator Transitions and Optical Dynamics. Unpublished report. (LA-UR-20-22985)

Presentation Slides

Klimov, V. I. Prospects & Challenges of Colloidal Quantum Dot Laser Diodes. . (LA-UR-21-24519)

Klimov, V. I. Semiconductor Nanocrystals: Tiny Particles with "Quantum Powers". . (LA-UR-21-24865)

Park, Y. Single-Particle Spectroscopy of Colloidal Quantum Dots. Presented at *Sungkyunkwan University Departmental Seminar (Online)*, Online, New Mexico, United States, 2021-05-19 - 2021-05-19. (LA-UR-21-24104)

Park, Y. Laser spectroscopy of colloidal quantum dots. Presented at *Job interview at Korea Advanced Institute of Science and Technology*, Daejun, Korea, South, 2021-05-26 - 2021-05-26. (LA-UR-21-24611)

Aging and Metastability of Delta-Phase Plutonium

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20210001DR

Project Description

Plutonium (Pu) is a remarkably complex element, and plutonium alloys exhibit similar complexity in their stability and physical properties. The latter is best and most importantly represented by phase relations within the plutonium-gallium system, with gallium being the most common alloying element for stabilizing delta-phase plutonium at room temperature. Despite intense international interest, the plutonium-gallium phase diagram is surprisingly controversial and lacks clear delineation of phase boundaries. This project will produce significant experimental and theoretical results that will greatly impact our fundamental understanding of Pu. Through integration of microstructure, thermophysical properties, and theory, we will produce a refined phase diagram that is both thermodynamically rigorous and aware of the kinetics of phase decomposition. En route to this larger goal, we will establish and employ novel state-of-the art tools that have yet to be used with Pu. These tools, and the results generated from them, will play critical roles in pushing the science of plutonium aging and manufacturing into the future.

Publications

Journal Articles

Rudin, S. P. Effects of substitutional Ga on the phonons of delta phase Pu based on density functional theory calculations. Submitted to *Physical Review B*. (LA-UR-21-30480)

Presentation Slides

Abdul-Jabbar, N. M. and J. N. Mitchell. Thermal Analysis of Preconditioned and Aged Pu-Ga Alloys. . (LA-UR-21-32015)

Barman, S. K. and S. C. Hernandez. A first-principles study on Ga stabilized \xce\xb4-Pu alloys. Presented at *APS March Meeting 2022*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22199)

Hernandez, S. C. Understanding an Unconventional Element Known as Plutonium. . (LA-UR-21-26157)

Manoj, A., S. C. Hernandez and M. N. Huda. Explaining the Properties of Plutonium with DFT. Presented at *Texas Section - APS*, Houston, Texas, United States, 2021-10-21 - 2021-10-21. (LA-UR-21-30405)

Mitchell, J. N., E. D. Bauer and S. C. Hernandez. 20210001DR Project Appraisal: Aging and Metastability of Delta-Phase Plutonium. Presented at *20210001DR LDRD Project Appraisal*, Los Alamos, New Mexico, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32087)

Olive, D. T. Challenges and Opportunities for Plutonium Science at Synchrotrons. Presented at *NSLS-II & CFN Joint Users' Meeting*, Upton, New York, United States, 2021-05-17 - 2021-05-20. (LA-UR-21-24655)

Rosa, P. Correlated f-electron materials: from quantum information to phase stability. Presented at *Materials Capability Review - LANL*, Los Alamos, New Mexico, United States, 2021-06-22 - 2021-06-22. (LA-UR-21-24716)

Rudin, S. P. Phonons as a means for understanding Pu-Ga materials. . (LA-UR-21-32114)

Rudin, S. P. How does Ga doping of \xce\xb4-Pu affect the phonons?. . (LA-UR-22-21688)

Tobash, P. H. Plutonium Materials Preparation and Processing in the New RLUOB Laboratory. . (LA-UR-21-32305)

Tutchton, R. M. Pseudopotential Development for Ab initio Molecular Dynamics. Presented at *20210001DR LDRD Project Appraisal*, Los Alamos, New Mexico, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32094)

Investigating How Material's Interfaces and Dislocations Affect Strength (iMIDAS)

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Project Description

The primary mission of Los Alamos National Laboratory (LANL) is stockpile stewardship, and every year LANL must certify that stockpile. In the absence of underground testing, the Laboratory uses modeling and simulation to make this assessment. However, like any mechanical instrument our stockpile is constantly evolving and undergoing changes due to internal and external environmental conditions and decisions by its caretakers. For example, materials age and new manufacturing methods become available. Such changes can lead to microstructural changes within materials and components, thus affecting the expected functionality. Currently, our codes cannot represent this change in properties due to the microstructure. To overcome this shortcoming, we must incorporate more physics into our models regarding the basic mechanisms that drive material yielding and hardening behavior, while keeping the computational cost low. We hypothesize that of known active deformation mechanisms, dislocation grain boundary interactions are one of the dominant mechanisms driving the overall material response. Hence, we plan to incorporate this mechanism into meso and macro-scale models within this project. Success of this project will result in a microstructurally aware macro-scale model available within the codes at LANL.

Publications

Journal Articles

W. Smith (Fey), L. T., A. Hunter and I. J. Beyerlein. Phase-field dislocation modeling of cross-slip. 2022. *Journal of Materials Science*. (LA-UR-21-28272 DOI: 10.1007/s10853-021-06716-1)

Gigax, J. G., E. Aydogan, S. S. Parker, B. P. Eftink, M. R. Chancey, J. Poplawsky and S. A. Maloy. Nitrogen content and radiation response in 12Cr ferritic/martensitic alloys. Submitted to *Scripta Materialia*. (LA-UR-21-29993)

Gigax, J. G., M. R. Chancey, H. Kim, Y. Wang, S. A. Maloy and N. Li. A novel microshear geometry for exploring the influence of void swelling on the mechanical properties induced by MeV heavy ion irradiation. Submitted to *Journal of Nuclear Materials*. (LA-UR-21-31405)

Harvey, C. R., A. J. Torrez, S. R. Lam, H. Kim, S. A. Maloy and J. G. Gigax. Demonstration of a high throughput tensile testing technique using femtosecond laser fabricated tensile bars in AISI 316 and additively manufactured grade 91 steel. Submitted to *JOM*. (LA-UR-21-26360)

*Pettes, M. T., A. Londono Calderon, D. J. Williams, B. H. Savitzky, C. Ophus, S. Ma, H. Zhu and M. M. Schneider. Intrinsic helical twist and chirality in ultrathin tellurium nanowires. 2021. *Nanoscale*. **13** (21): 9606-9614. (LA-UR-21-21904 DOI: 10.1039/D1NR01442K)

Pettes, M. T., A. Londono Calderon, R. Dhall, C. Ophus, Y. Wang, E. Dervishi-Whetham, H. S. Kang, C. Lee and J. Yoo. Visualizing Grain Statistics in MOCVD WSe through Four-Dimensional Scanning Transmission Electron Microscopy. 2022. *Nano Letters*. (LA-UR-21-30267 DOI: 10.1021/acs.nanolett.1c04315)

Tavenner, J. P., A. Gupta, G. B. Thompson, E. M. Kober and G. J. Tucker. Advanced Structural Descriptors for Predicting Segregation Potential: Fingerprinting Grain Boundary Atomic Environments. Submitted to *NPJ Computational Materials*. (LA-UR-21-20647)

Tavenner, J. P., A. Gupta, G. B. Thompson, E. M. Kober and G. J. Tucker. Fingerprinting Complex Atomic Environments: Learning Local Segregation Energy Behavior at Grain Boundaries. Submitted to *NPJ Computational Materials*. (LA-UR-21-30331)

Xie, D., M. Chen, J. G. Gigax, M. Zikry, D. J. Luscher, A. Hunter, S. J. Fensin and N. Li. In situ pillar compression to explore the strain hardening mechanisms in single crystal Cu. Submitted to *Scripta Materialia*. (LA-UR-21-31596)

Reports

Kober, E. M., R. Vangara, N. K. Rai and B. Alexandrov. Integrated Learning of High Explosives Initiation Processes. Unpublished report. (LA-UR-21-21148)

Peng, X., L. T. Fey, H. Kim, A. Hunter and E. Martinez. PFDD CPP Manual. Unpublished report. (LA-UR-21-31582)

Presentation Slides

Adams, C. M., J. P. Tavenner, N. Mathew and E. M. Kober. Characterizing Atomistic Geometries and Potential Functions Using Strain Functionals. Presented at *TMS2021 Annual Meeting*, Orlando, Florida, United States, 2021-03-14 - 2021-03-14. (LA-UR-21-22385)

Chakraborty, S., A. Hunter and D. J. Luscher. Development of dislocation transport-based macroscale crystal plasticity model. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-03-01 - 2022-03-08. (LA-UR-22-21932)

Chen, J., K. Q. Dang, H. T. Vo, P. Hosemann and S. J. Fensin. Associating GB Characteristics with its Sink Efficiency in Absorbing Frank Loops in Cu. Presented at *PASC -- virtual*, Geneva, Switzerland, 2021-07-05 - 2021-07-08. (LA-UR-21-27827)

Gigax, J. G. Mesopillar Compression of Cu (Set B). . (LA-UR-21-30703)

Gigax, J. G., H. Kim and M. M. Schneider. Using fully convolution neural networks for image segmentation. . (LA-UR-21-29953)

Li, N. In Situ Nanomechanical Testing to Explore the Impact of Grain Boundaries on Mechanical Properties. Presented at *Materials Capability Review*, Los Alamos, New Mexico, United States, 2021-06-21 - 2021-06-21. (LA-UR-21-24884)

Li, N., D. Xie, J. G. Gigax, S. Athikavil Suresh, R. Pokharel, S. J. Fensin, X. Peng, A. Hunter, M. Chen and M. Zikry. Novel in situ strain mapping via high resolution EBSD in a SEM to understand dislocation-dislocation and dislocation-grain boundary interactions. Presented at *FY22 DR Appraisal*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-06. (LA-UR-21-31726)

Li, N., D. Xie, S. J. Fensin, A. Hunter, D. J. Luscher, M. Chen and M. Zikry. In situ nanomechanical testing to understand dislocation-dislocation and dislocation-grain boundary interactions. Presented at *TMS 2022 Annual Meeting & Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-03-03. (LA-UR-22-21596)

Parida, S., Y. Wang, H. Zhao, H. Htoon, T. Choudhury, J. Redwing, A. Dongare and M. T. Pettes. Mechanical Tuning of the Electronic and Vibrational Properties of Epitaxial MoS2 through Ion Beam Modification. Presented at *2021 MRS Fall Meeting & Exhibit*, Boston, Massachusetts, United States, 2021-11-29 - 2021-11-29. (LA-UR-21-31636)

Peng, X., E. Martinez, N. Mathew, D. J. Luscher, A. Hunter and I. J. Beyerlein. A combined kinetic Monte Carlo and phase field approach to modeling thermally activated dislocation motion. Presented at *TMS 2022 Annual Meeting & Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-22050)

Peng, X., E. Martinez, N. Mathew, D. J. Luscher, A. Hunter and I. J. Beyerlein. A combined kinetic Monte Carlo and phase field approach to modeling thermally activated dislocation motion. Presented at *TMS 2022 Annual Meeting & Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-22170)

Pettes, M. T. Towards control over 2D material properties through ion beam modification and analysis. Presented at *CINT 2021 Annual Meeting*, Online, New Mexico, United States, 2021-09-21 - 2021-09-21. (LA-UR-21-29318)

Pettes, M. T. Emergent Phenomena in van der Waals Materials: Advancements in Characterization. Presented at *Invited talk at University of Southern California*, Los Angeles, California, United States, 2021-05-28 - 2021-05-28. (LA-UR-21-31292)

Athikavil Suresh, S., K. Q. Dang, M. I. Baskes, E. M. Kober, N. Mathew, A. Hunter and S. J. Fensin. High-throughput Atomistic Simulations of Dislocation-Grain Boundary interactions. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-28 - 2022-03-03. (LA-UR-22-21674)

Xie, D., M. Chen, M. Zikry, J. G. Gigax, N. Mathew, D. J. Luscher, A. Hunter, S. J. Fensin and N. Li. Investigation of Dislocation-grain Boundary Interactions in a Cu-1%Pb Alloy through In-situ Micro-mechanical Testing with High Resolution EBSD. Presented at *TMS 2022 Annual Meeting & Exhibition*, anaheim, California, United States, 2022-02-27 - 2022-03-03. (LA-UR-22-21468)

Other

Gigax, J. G., N. Li, S. J. Fensin and A. Hunter. Initial mesoscale tensile testing in polycrystalline Cu. Dataset. (LA-UR-21-26004)

Topological Quantum Materials for Robust Quantum Computing

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Project Description

A quantum computer performs calculations based on the quantum superposition of different states and holds the promise of solving several classes of problems that are intractable using classical computers. Current quantum computers are built upon quantum two-level systems, such as superconducting qubits; however, the bottleneck preventing quantum computers from solving real-world problems is their short coherence time, i.e., the time scale in which a qubit loses quantum coherence. A fundamentally new paradigm based on novel excitations in topological quantum materials that harnesses the robustness of certain quantum materials can be exploited to achieve fault-tolerant quantum computation. We will develop a materials platform for future quantum computers based on topological quantum materials. We will use the most promising routes to achieve quantum ground states supporting Majorana fermions (MFs), namely topological superconductivity and quantum spin liquid states. Our goals are to establish design principles and provide new materials platforms that host MFs and to develop a combination of probes for unambiguously identifying MFs.

Publications

Journal Articles

Banerjee, S., U. Kumar and S. Lin. Inverse Faraday effect in Mott insulators. Submitted to *Physical Review Letters*. (LA-UR-21-28801)

*Duan, C., K. Sasmal, M. B. Maple, A. Podlesnyak, J. Zhu, Q. Si and P. Dai. Incommensurate Spin Fluctuations in the Spin-triplet Superconductor Candidate UTe2. 2020. *Physical Review Letters*. **125** (23): 237003. (LA-UR-20-24870 DOI: 10.1103/PhysRevLett.125.237003)

Huang, Z., C. S. Ting, J. Zhu and S. Lin. Gapless Higgs Mode in the Fulde-Ferrell-Larkin-Ovchinnikov State of a Superconductor. Submitted to *Physical Review Letters*. (LA-UR-21-24876)

Lane, C. A., L. Chen, H. Hu, E. Nica, J. Zhu and Q. Si. Multiorbital spin-triplet pairing and spin resonance in the heavy fermion superconductor UTe2. Submitted to *Physical Review Letters*. (LA-UR-21-32485)

Li, H., U. Kumar, K. Sun and S. Lin. Spontaneous fractional Chern insulators in transition metal dichacogenides Moir \xc3\xa9 superlattices. Submitted to *Physical Review Letters*. (LA-UR-21-20020)

Lin, S. Skyrmion lattice in centrosymmetric magnets with local Dzyaloshinsky-Moriya interaction. Submitted to *Scipost Physics*. (LA-UR-21-32483)

Malla, R. K. Nonadiabatic dissociation of molecular condensates: competition between multi-mode reaction channels. Submitted to *Physical Review Letters*. (LA-UR-22-21329)

Malla, R. K., V. Y. Chernyak, C. Sun and N. Sinitsyn. Coherent reaction between molecular and atomic Bose-Einstain condensates: integrable model. Submitted to *Physical Review Letters*. (LA-UR-21-32402)

Mukkattu Omanakuttan, A., S. M. Thomas, S. K. Kushwaha, E. D. Bauer, F. Ronning, J. D. Thompson, N. Harrison and P. Rosa. Ground state of Ce3Bi4Pd3 unraveled by hydrostatic pressure. Submitted to *Physical Review Letters*. (LA-UR-21-30470)

Rosa, P., A. C. Weiland, S. S. Fender, B. L. Scott, F. Ronning, J. D. Thompson, E. D. Bauer and S. M. Thomas. Single-component superconducting state in UTe2 at 2 K. Submitted to *Nature Communications*. (LA-UR-21-30149)

Saitou, Y., N. Ichikawa, R. Yamamoto, D. Kitamata, M. Suzuki, Y. Yanagita, T. Namaizawa, S. Komuro, T. Furukawa, R. Kato and T. Itou. Unconventional superconductivity exhibiting Pauli spin paramagnetism in an organic triangular-lattice Mott system. Submitted to *Nature Physics*. (LA-UR-21-31854)

*Schoenemann, R., S. Imajo, F. Weickert, J. Yan, D. G. Mandrus, Y. Takano, E. L. Brosha, P. F. S. Rosa, S. E. Nagler, K. Kindo and M. Jaime. Thermal and magnetoelastic properties of in the field-induced low-temperature states. 2020. *Physical Review B*. **102** (21): 214432. (LA-UR-20-23885 DOI: 10.1103/PhysRevB.102.214432)

Sinitsyn, N., A. Fisher, I. Kleinjoharnn and F. B. Anders. Cross-correlation spectra in interacting quantum dot systems. Submitted to *Physical Review B*. (LA-UR-21-28148)

Thomas, S. M., C. Stevens, F. B. Santos, S. S. Fender, E. D. Bauer, F. Ronning, J. D. Thompson, A. Huxley and P. Rosa. Spatially inhomogeneous superconductivity in. 2021. *Physical Review B*. **104** (22): 224501. (LA-UR-21-22477 DOI: 10.1103/PhysRevB.104.224501)

Xu, C., C. Cao and J. Zhu. Pressure-induced concomitant topological and metal-insulator quantum phase transitions in Ce3Pd3Bi4. Submitted to *Nature Communications*. (LA-UR-21-28777)

*Zhentao, W., S. Ying, L. Shi-Zeng and C. D. Batista. Meron, skyrmion, and vortex crystals in centrosymmetric tetragonal magnets. 2021. *Physical Review B*. **103** (10): 104408. (LA-UR-20-29175 DOI: 10.1103/PhysRevB.103.104408)

Presentation Slides

Bordelon, M. M., C. P. M. Girod, S. M. Thomas, J. D. Thompson, E. D. Bauer and P. Rosa. Unusual antiferromagnetism and field-induced transitions in tetragonal CeLiBi2. Presented at *International Conference on Strongly Correlated Electron Systems*, Campinas, Brazil, 2021-09-27 - 2021-10-02. (LA-UR-21-28184)

Coker, A. A. Spin Dynamics in the Kagome Lattice. Presented at *2021 LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27684)

Lin, S. Enhanced superconductivity in quasiperiodic systems. Presented at *APS March Meeting*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-20. (LA-UR-21-22478)

Malla, R. K. Coherent reaction between molecular and atomic Bose-Einstein condensates\xc2\xa0. Presented at *University of Massachusetts, Lowell*, Lowell, Massachusetts, United States, 2022-02-25 - 2022-02-25. (LA-UR-22-21677)

Malla, R. K. Ultrafast dynamics in Kane-Mele two-dimensional topological insulators. Presented at *APS March meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-14. (LA-UR-22-21966)

Martin, M. J. Quantum information science with Rydberg atoms. . (LA-UR-20-29116)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *UNM CQuIC seminar*, Albuquerque, New Mexico, United States, 2021-02-04 - 2021-02-04. (LA-UR-21-20920)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *LANL/TAMU Quantum Seminar Series*, College Station, Texas, United States, 2021-04-27 - 2021-04-27. (LA-UR-21-23972)

Martin, M. J. Quantum information science and sensing with ultracold neutral atoms. . (LA-UR-21-25997)

Martin, M. J. Quantum information science with laser-dressed atoms Q-SEnSE Convergence Seminar. Presented at *Q-SEnSE Convergence Seminar*, Boulder, Colorado, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32107)

Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

Rosa, P. Correlated f-electron materials: from quantum information to phase stability. Presented at *Materials Capability Review - LANL*, Los Alamos, New Mexico, United States, 2021-06-22 - 2021-06-22. (LA-UR-21-24716)

Rosa, P., S. M. Thomas, C. P. M. Girod, J. D. Thompson and E. D. Bauer. Unusual magnetism and field-induced transitions in Cerium-based materials. Presented at *New directions in strong correlation physics: From strange metals to topological superconductivity*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-28. (LA-UR-22-20362)

Weiland, A. C., S. S. Fender, F. Ronning, J. D. Thompson, E. D. Bauer, S. M. Thomas and P. Rosa. Correlating Tc and Crystallographic Parameters in UTe2. Presented at *Chirality, Topology, and Unconventional Superconductivity in Sr2RuO4 and UTe2*, Santa Fe, New Mexico, United States, 2021-10-28 - 2021-10-30. (LA-UR-21-30512)

Weiland, A. C., S. S. Fender, M. M. Bordelon, F. Ronning, J. D. Thompson, E. D. Bauer, S. M. Thomas and P. Rosa. The Effects of Annealing in UTe2. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-15 - 2022-03-19. (LA-UR-22-22016)

Posters

M. Girod, C. P., S. M. Thomas, P. Rosa, F. Ronning, E. D. Bauer, J. D. Thompson, A. Huxley and C. Stevens. Mapping superconductivity with uniaxial stress in UTe2. Presented at *2022 Aspen Winter Conference, New Directions in Strong Correlation Physics: From Strange Metals to Topological Superconductivity*, Aspen, Colorado, United States, 2022-01-24 - 2022-01-28. (LA-UR-22-20243)

Weiland, A. C., P. Rosa, S. S. Fender, B. L. Scott, F. Ronning, J. D. Thompson, E. D. Bauer and S. M. Thomas. A Crystallographic Study of UTe2. Presented at *NEW DIRECTIONS IN STRONG CORRELATION PHYSICS: FROM STRANGE METALS TO TOPOLOGICAL SUPERCONDUCTIVITY*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-29. (LA-UR-22-20422)

Uncovering the Role of 5f-electron Magnetism in the Electronic Structure and Equation of State of Plutonium (U)

Neil Harrison
20180025DR

Project Description

Accurate simulations of plutonium under extreme conditions require an accurate knowledge of the electronic structure and equation of state. Magnetism is presently a missing component of the electronic structure and equation of state that is known to have a significant influence on the equilibrium volume, bulk modulus and other properties. The goal of the present project is to determine primarily by way of experiment, accompanied by advanced theoretical modeling tools, the correct way of incorporating the effects of magnetism in the electronic structure and equation of state of plutonium. The end result will be an accurate understanding of the mechanism at play when delta-plutonium undergoes its initial volume collapse at low pressure. Such an understanding is crucial for accurate estimates to be made of plutonium's physical quantities under reduced volume, and also by extrapolation into more extreme environments where accurate or safe measurements are presently not possible.

Technical Outcomes

The electronic energy scale associated with the electronic structure of delta-plutonium is roughly an order of magnitude lower than has been predicted based on any of the electronic structure models. This project confirmed this using two different experiments — magnetostriction and heat capacity measurements — as well as the most comprehensive dynamical mean field theory (DMFT) calculations of the electronic structure performed thus far. Though DMFT is somewhat realistic, it is not yet able to account for the small energy scales.

Publications

Journal Articles

*Balakirev, F. F., S. M. Ennaceur, R. J. Migliori and A. Migliori. Resonant ultrasound spectroscopy: The essential toolbox. 2019. *Review of Scientific Instruments*. **90** (12): 121401. (LA-UR-19-28447 DOI: 10.1063/1.5123165)

*Harrison, N. Electronically driven collapse of the bulk modulus in -plutonium. 2020. *Proceedings of the National Academy of Sciences of the United States of America*. **117** (9): 4480-4485. (LA-UR-19-32035 DOI: 10.1073/pnas.1918281117)

Harrison, N., J. B. Betts, F. F. Balakirev, S. Richmond, M. Jaime and P. H. Tobash. Twin source of electronic disorder in plutonium. Submitted to *TBD*. (LA-UR-19-20229)

Harrison, N., M. R. Wartenbe, P. H. Tobash, J. Singleton, L. E. W. Stritzinger and S. Richmond. Pseudogap in elemental plutonium. Submitted to *Nature Physics*. (LA-UR-20-24656)

Harrison, N. and M. Jaime. Hidden valence transition in uranium ruthenium two silicon two. Submitted to *Nature Communications*. (LA-UR-19-21055)

Harrison, N. and P. H. Tobash. Resolution to the missing entropy at the delta - alpha volume collapse in Pu-Ga alloys. Submitted to *Physical Review*. (LA-UR-20-24241)

Joyce, J. J., K. S. Graham, J. Zhu, G. H. Lander, T. Durakiewicz, J. M. Wills, P. H. Tobash, E. D. Bauer, J. N. Mitchell and H. Choi. Competing Electronic Configurations for PuTe and New Insight on Plutonium Metal. Submitted to *Physical Review Letters*. (LA-UR-19-20178)

*Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. F. S. Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Nature Communications*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

Tutchton, R. M., W. Chiu, R. C. Albers, G. Kotliar and J. Zhu. Supplementary Information: Electronic Correlation Induced Expansion of Compensated Electron and Hole Fermi Pockets in d-Plutonium. Submitted to *Nature Communications*. (LA-UR-19-29905)

*Tutchton, R. M., W. Chiu, R. C. Albers, G. Kotliar and J. Zhu. Electronic Correlation Induced Expansion of Fermi Pockets in delta-Plutonium. 2020. *Physical Review B*. **101** (24): 245156. (LA-UR-19-29904 DOI: 10.1103/PhysRevB.101.245156)

Conference Papers

Harrison, N., J. B. Betts, P. H. Tobash and M. Jaime. Magnetostriction of Ga-stabilized delta-plutonium. Presented at *Plutonium Futures*. (San Diego, California, United States, 2018-09-09 - 2018-09-14). (LA-UR-18-26836)

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the electronic and magnetic structure of Pu6Fe. Presented at *Pu Futures 2018*. (San Diego, California, United States, 2018-09-09 - 2018-09-09). (LA-UR-18-23453)

Maiorov, B. A., J. B. Betts, F. F. Balakirev and A. Migliori. Temperature dependent and Real Time Studies of Elastic Moduli of \xce\xb4-239Pu and alloys. Presented at *Plutonium Futures*. (san diego, California, United States, 2018-09-09 - 2018-09-14). (LA-UR-18-25818)

Tobash, P. H., E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, S. Richmond, D. Wheeler and T. Albrecht-Schmitt. Progress on the Thermophysical Properties of Some Plutonium Alloys and Compounds. Presented at *Pu Futures 2018*. (San Diego, California, United States, 2018-09-09 - 2018-09-09). (LA-UR-18-23371)

Books/Chapters

Tobash, P. H. and S. Bobev. Chemical Bonding and Structural Relationships in Extended Solids. (LA-UR-18-28530)

Reports

Nelson, C. A. Uncovering the role of 5f-electron magnetism in plutonium using capacitive dilatometry. Unpublished report. (LA-UR-19-20411)

Presentation Slides

Harrison, N. Magnetostriction of delta-plutonium. Presented at *Plutonium futures*, san diego, California, United States, 2018-09-09 - 2018-09-09. (LA-UR-18-28499)

Harrison, N. Magnetostriction of delta plutonium 2. Presented at *Plutonium Futures*, San Diengo, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28630)

Harrison, N., P. H. Tobash, M. Jaime, S. Richmond, J. B. Betts and M. R. Wartenbe. Phase stabilization by electronic entropy in plutonium. Presented at *American Physical Society March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21885)

Hernandez, S. C. Insights into point-defects of \xce\xb4-Pu and \xce\xb4-Pu-Ga alloys using density functional theory. Presented at *Uppsala University*, Uppsala, Sweden, 2018-06-08 - 2018-06-08. (LA-UR-18-24654)

Hernandez, S. C. Overview of using density functional theory for material science applications on Pu and its compounds. Presented at *Computational Data Science Approaches for Materials*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23136)

Hernandez, S. C. Density functional theory study of aging of Pu. . (LA-UR-20-21880)

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the Electronic and Magnetic Structure of Pu6Fe. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21830)

Kushwaha, S. K., M. K. Chan, N. Harrison, P. Ferrari Silveira Rosa, S. M. Thomas, E. D. Bauer, F. Ronning, J. Park and J. D. Thompson. Magnetic field induced Fermi liquid in a candidate topological Kondo insulator. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22244)

Maiorov, B. A., J. B. Betts, F. F. Balakirev, F. J. Freibert and A. Migliori. Temperature Dependent and Real Time Studies of Elastic Moduli of \xce\xb4-239Pu and Alloys. Presented at *Plutonium Futures*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-29991)

Migliori, A. and S. M. Ennaceur. Toward an understanding of aging in plutonium from direct measurements of stored energy. . (LA-UR-18-31769)

Tobash, P. H., E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, T. Albrecht-Schmitt and D. Wheeler. Thermophysical Property Studies on Pu Alloys and Compounds. Presented at *MRS 2018*, Phoneix, Arkansas, United States, 2018-04-02 - 2018-04-02. (LA-UR-18-22563)

Tobash, P. H., S. Richmond, E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, D. Wheeler and T. Albrecht-Schmitt. Progress on the Thermophysical Properties of Some Plutonium Alloys and Compounds. Presented at *Pu Futures 2018*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28267)

Tutchton, R. M. Correlation and Electron-phonon coupling in the Electronic structure of Plutonium. Presented at *Science in 3*, Los Alamos, New Mexico, United States, 2018-06-13 - 2018-06-13. (LA-UR-18-26227)

Tutchton, R. M., J. Julien, Q. Si and J. Zhu. First Principles Study of the Fermi Surface Topology of CeCu2Si2. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22188)

Tutchton, R. M., J. Julien, Q. Si and J. Zhu. First Principles Study of the Fermi Surface Topology of CeCu2Si2. Presented at *Quantum Mater and Beyond*, Jacksonville, Florida, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-31974)

Tutchton, R. M., J. Zhu and W. Chiu. Data Diversity as a Tool In the Search for d-Pu's Missing Magnetism. Presented at *Computational Data Science Approaches for Materials*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-26601)

Tutchton, R. M., W. C. Chiu, G. Resta, T. Lee, E. D. Bauer, F. Ronning, R. T. Scalettar and J. Zhu. Hybridization effect on the X-ray absorption spectra for actinide materials. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-14. (LA-UR-22-21518)

Tutchton, R. M. and J. Zhu. Fermi Surface Topology and Correlation Effects in the Electronic Structure of Plutonium. Presented at *APS March meeting*, Boston, Massachusetts, United States, 2019-03-03 - 2019-03-08. (LA-UR-19-21868)

Wartenbe, M. R., P. H. Tobash, N. Harrison, J. B. Betts, J. Singleton and L. E. W. Stritzinger. Plutonium in high magnetic fields. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22254)

Posters

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the Electronic and Magnetic Structure of Pu6Fe. Presented at *Pu Futures 2018*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28384)

Nelson, C. A., M. R. Wartenbe, S. M. Thomas, G. M. Schmiedeshoff, N. Harrison and P. H. Tobash. Assembling and Calibrating a Capacitive Dilatometer for Magnetostriction and Thermal Expansion Measurements. . (LA-UR-18-26970)

Richmond, S. (U) Plutonium sample processing, grain growth and extraction by hydriding. . (LA-UR-19-21170)

Tutchton, R. M. and J. Zhu. Fermi Surface Topology and Correlation Effects in the Electronic Structures of Plutonium. Presented at *LRDR review*, Los Alamos, New Mexico, United States, 2019-02-26 - 2019-02-26. (LA-UR-19-21439)

Tutchton, R. M. and J. Zhu. Temperature Dependent Phonon Dispersions of Non-magnetic delta-Plutonium. Presented at *Theory Frontiers in Actinide Sciences: Chemistry and Materials*, Santa Fe, New Mexico, United States, 2020-02-02 - 2020-02-05. (LA-UR-20-20745)

Rational Design of Halide Perovskites for Next Generation Gamma-ray Detection

Sergei Tretiak
20180026DR

Project Description

This project will address two key national security challenges: (i) we will establish the scientific understanding and the design principles for a new halide perovskite materials technology for the fabrication of radiation detectors, critical for several Los Alamos National Laboratory and NNSA missions; (ii) we will demonstrate a proof-of-concept room temperature (RT) operated gamma ray detector with sensitivity and energy resolution exceeding that of cadmium-zinc-telluride (CZT) detectors, which represent the state-of-the-art for RT Gamma-ray detection.

Technical Outcomes

Through this project, experimental and computational scientists have worked closely to investigate new perovskite structures and surface and interface properties to design new materials suitable for gamma-ray detectors and beyond. We have synthesized a number of new perovskite materials, which were successfully tested in the detector devices. Some results were groundbreaking, such as for X-ray detection. The Los Alamos team became an established world-leader in the area of halide perovskite materials.

Publications

Journal Articles

*Appavoo, K., W. Nie, J. -. Blancon, J. Even, A. D. Mohite and M. Y. Sfeir. Ultrafast optical snapshots of hybrid perovskites reveal the origin of multiband electronic transitions. 2017. *Physical Review B*. **96** (19): 195308. (LA-UR-17-29873 DOI: 10.1103/PhysRevB.96.195308)

*Blancon, J. -., A. V. Stier, H. Tsai, W. Nie, C. C. Stoumpos, B. Traore, L. Pedesseau, M. Kepenekian, F. Katsutani, G. T. Noe, J. Kono, S. Tretiak, S. A. Crooker, C. Katan, M. G. Kanatzidis, J. J. Crochet, J. Even and A. D. Mohite. Scaling law for excitons in 2D perovskite quantum wells. 2018. *Nature Communications*. **9** (1): 2254. (LA-UR-18-30029 DOI: 10.1038/s41467-018-04659-x)

Blancon, J. R., A. V. Stier, H. Tsai, W. Nie, C. Stoumpos, B. Traore, L. Pedesseau, M. Kepenekian, S. Tretiak, S. A. Crooker, C. Katan, M. G. Kanatzidis, J. J. Crochet, A. Mohite and J. Even. Strongly bound excitons in Ruddlesden-Popper 2D perovskites. Submitted to *arXiv*. (LA-UR-17-29656)

Canicoba, N., N. Zagni, F. Liu, K. Fernando, H. Belleza, B. Traor \xc3\xa9, R. Rogel, H. Tsai, L. L. Brizoual, W. Nie, J. J. Crochet, S. Tretiak, C. Katan, J. Even, M. Kanatzidis, B. W. Alphenaar, J. C. Blancon, M. A. Alam and A. D. Mohite. Halide Perovskite High-k Field Effect Transistors with Dynamically Reconfigurable Ambipolarity. 2019. *ACS materials letters*. **1** (6): 633-640. (LA-UR-19-28793 DOI: 10.1021/acsmaterialslett.9b00357)

*Collins, L., E. S. Muckley, H. Tsai, D. Ghosh, A. J. Neukirch, S. Tretiak, S. V. Kalinin, W. Nie and I. N. Ivanov. Correlation of Spatiotemporal Dynamics of Polarization and Charge Transport in Blended Hybrid Organic–Inorganic Perovskites on Macro- and Nanoscales. 2020. *ACS Applied Materials & Interfaces*. **12** (13): 15380-15388. (LA-UR-19-28377 DOI: 10.1021/acsami.0c00561)

Fernando, K., C. N. Devesa, J. C. Blancon, H. Tsai, J. Even, P. M. Ajayan, M. G. Kanatzidis, M. A. Alam, W. Nie, B. W. Alphenaar and A. D. Mohite. Origin of intrinsic unipolar memristors action on a single-grain of halide perovskite. Submitted to *Nature Communications*. (LA-UR-19-20524)

Ghosh, D., P. Parida and S. Pati. A small heterocyclic molecule as a multistate transistor: a quantum many-body approach. 2021. *Journal of Materials Chemistry C*. **9** (33): 10927-10934. (LA-UR-21-25700 DOI: 10.1039/D1TC01092A)

Huang, H., H. Tsai, R. Raja, S. Lin, D. Ghosh, C. Hou, J. Shyue, C. Chang, S. Tretiak, W. Chen, W. Nie, K. Lin and L. Wang. Robust un-encapsulated perovskite solar cells protected by fluorinated fullerene electron transporting layer. Submitted to *Nature*. (LA-UR-20-23214)

Huang, H., Q. Liu, H. Tsai, S. Shrestha, l. Su, P. Chen, Y. Chen, H. Lu, C. Chuang, K. Lin, S. Rwei, W. Nie and L. Wang. A simple one-step method with wide processing window for high quality perovskite mini-module fabrication. Submitted to *Advanced Energy Materials*. (LA-UR-20-27549)

Jenen, K. L., A. Shabaev, S. G. Lambrakos, D. Finkenstadt, A. J. Neukirch, N. A. Moody, S. Tretiak, D. A. Shiffler and J. J.

Petillo. Analytic Model of Electron Transport Through and Over Non-Linear Barriers. Submitted to *Journal of Applied Physics*. (LA-UR-20-22694)

Jensen, K. L., A. Shabaev, S. G. Lambrakos, D. Finkenstadt, J. J. Petillo, A. J. Neukirch, A. M. Alexander, J. M. Smedley, N. A. Moody, H. Yamaguchi, F. Liu and S. Tretiak. An Extended Moments Model of Quantum Efficiency for Metals and Semiconductors. Submitted to *New Journal of Physics*. (LA-UR-20-23027)

*Kepenekian, M., B. Traore, J. Blancon, L. Pedesseau, H. Tsai, W. Nie, C. C. Stoumpos, M. G. Kanatzidis, J. Even, A. D. Mohite, S. Tretiak and C. Katan. Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. 2018. *Nano Letters*. **18** (9): 5603-5609. (LA-UR-18-20158 DOI: 10.1021/acs.nanolett.8b02078)

Kinigstein, E. D., H. Tsai, W. Nie, J. Blancon, K. G. Yager, K. Appavoo, J. Even, M. G. Kanatzidis, A. D. Mohite and M. Y. Sfeir. Edge States Drive Exciton Dissociation in Ruddlesden–Popper Lead Halide Perovskite Thin Films. 2020. *ACS Materials Letters*. **2** (10): 1360-1367. (LA-UR-20-21239 DOI: 10.1021/acsmaterialslett.0c00333)

*Kobbekaduwa, K., S. Shrestha, P. Adhikari, E. Liu, L. Coleman, J. Zhang, Y. Shi, Y. Zhou, Y. Bekenstein, F. Yan, A. M. Rao, H. Tsai, M. C. Beard, W. Nie and J. Gao. In-situ observation of trapped carriers in organic metal halide perovskite films with ultra-fast temporal and ultra-high energetic resolutions. 2021. *Nature Communications*. **12** (1): 1636. (LA-UR-20-27180 DOI: 10.1038/s41467-021-21946-2)

Leveillee, J. A., C. Katan, J. Even, A. Mohite, S. Tretiak, A. Schleife and A. J. Neukirch. First principles survey of organic spacer candidates for tuned light emission from layered hybrid perovskite materials. Submitted to *ACS Energy Letters*. (LA-UR-19-20225)

*Leveillee, J., C. Katan, L. Zhou, A. D. Mohite, J. Even, S. Tretiak, A. Schleife and A. J. Neukirch. Influence of -conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. 2018. *Physical Review Materials*. **2** (10): 105406. (LA-UR-18-22811 DOI: 10.1103/PhysRevMaterials.2.105406)

. G. D. *. J. K. L. *. F. D. *. S. A. *. L. S. G. *. L. F. *. N. W. *. B. J. *. Z. L. *. C. J. J. *. M. N. *. M. A. D. *. T. S. *. N. A. J. Lewis, S. G., S. G. Lewis, D. Ghosh, F. Liu, W. Nie, L. Zhou, J. J. Crochet, S. Tretiak, A. J. Neukirch and N. Moody. Cesium-Coated Halide Perovskites as a Photocathode Material: Modeling Insights. 2021. *The Journal of Physical Chemistry Letters*. **12 (27): 6269-6276. (LA-UR-21-24212 DOI: 10.1021/acs.jpclett.1c01412)

Lewis, S. G., F. Liu, W. Nie, L. Zhou, N. A. Moody, A. Mohite, S. Tretiak and A. J. Neukirch. Cesium coated halide perovskites as new photocathode material. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-20077)

*Li, X., J. Hoffman, W. Ke, M. Chen, H. Tsai, W. Nie, A. D. Mohite, M. Kepenekian, C. Katan, J. Even, M. R. Wasielewski, C.

C. Stoumpos and M. G. Kanatzidis. Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, (NH3CmH2mNH3)(CH3NH3)(n-1)PbnI3n+1 (m=4-9; n=1-4). 2018. *Journal of the American Chemical Society*. **140** (38): 12226-12238. (LA-UR-19-20437 DOI: 10.1021/jacs.8b07712)

*Liu, C., H. Tsai, W. Nie, D. J. Gosztola and X. Zhang. Direct Spectroscopic Observation of the Hole Polaron in Lead Halide Perovskites. 2020. *The Journal of Physical Chemistry Letters*. **11** (15): 6256-6261. (LA-UR-20-24148 DOI: 10.1021/acs.jpclett.0c01708)

Liu, F., M. A. Hoffbauer, S. G. Lewis, A. J. Neukirch, V. Pavlenko, H. Tsai, W. Nie, P. M. Ajayan, M. Kanatzidis, J. J. Crochet, N. A. Moody, J. R. Blancon and A. Mohite. Highly-efficient and regenerative electron sources using halide perovskite semiconductor thin films. Submitted to *Science*. (LA-UR-19-32662)

*Liu, F., M. Yoho, H. Tsai, K. Fernando, J. Tisdale, S. Shrestha, J. K. Baldwin, A. D. Mohite, S. Tretiak, D. T. Vo and W. Nie. The working principle of hybrid perovskite gamma-ray photon counter. 2020. *Materials Today*. **37**: 27-34. (LA-UR-19-25920 DOI: 10.1016/j.mattod.2020.02.022)

Liu, F., S. G. Lewis, A. J. Neukirch, V. Pavlenko, M. A. Hoffbauer, H. Tsai, W. Nie, J. Even, S. Tretiak, M. G. Kanatzidis, J. J. Crochet, N. A. Moody, J. C. Blancon and A. D. Mohite. Highly-efficient and regenerative electron sources using halide perovskite semiconductor thin films. Submitted to *Science*. (LA-UR-19-32491)

Neukirch, A. J., D. Ghosh, D. Acharya, L. Zhou, W. Nie, O. V. Prezhdo and S. Tretiak. Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-28376)

Neukirch, A. J., D. Ghosh, L. Zhou, O. Prezhdo and S. Tretiak. Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Submitted to *ACS Energy Letters*. (LA-UR-19-26479)

*Neukirch, A. J., I. I. Abate, L. Zhou, W. Nie, H. Tsai, L. Pedesseau, J. Eyen, J. J. Crochet, A. D. Mohite, C. Katan and S. Tretiak. Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. 2018. *The Journal of Physical Chemistry Letters*. **9** (24): 7130-7136. (LA-UR-18-30565 DOI: 10.1021/acs.jpclett.8b03343)

Neukirch, A. J., J. A. Leveillee, J. Even, D. Ghosh, W. Nie, A. Mohite, S. Tretiak and A. Schleife. Tuning electronic structure in layered hybrid perovskites with organic spacer substitution. Submitted to *Nano Letters*. (LA-UR-19-28375)

Park, M., A. J. Neukirch, S. E. Reyes-Lillo, M. Lai, S. Ellis, D. Dietze, J. Neaton, P. Yang, S. Tretiak and R. Mathies. Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. Submitted to *Nature Communications*. (LA-UR-18-25906)

*Park, M., A. J. Neukirch, S. E. Reyes-Lillo, M. Lai, S. R. Ellis, D. Dietze, J. B. Neaton, P. Yang, S. Tretiak and R. A. Mathies. Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. 2018. *Nature Communications*. **9** (1): 2525. (LA-UR-17-31256 DOI: 10.1038/s41467-018-04946-7)

Mora Perez, C., A. J. Neukirch, D. Ghosh, O. V. Prezhdo and S. Tretiak. Excited-state Properties of Defected Halide Perovskite Quantum Dots: Insights from Computation. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-20-28950)

*Rolston, N., A. D. Printz, J. M. Tracy, H. C. Weerasinghe, D. Vak, L. J. Haur, A. Priyadarshi, N. Mathews, D. J. Slotcavage, M. D. McGehee, R. E. Kalan, K. Zielinski, R. L. Grimm, H. Tsai, W. Nie, A. D. Mohite, S. Gholipour, M. Saliba, M. Gratzel and R. H. Dauskardt. Effect of Cation Composition on the Mechanical Stability of Perovskite Solar Cells. 2018. *Advanced Energy Materials*. **8** (9): 1702116. (LA-UR-18-30108 DOI: 10.1002/aenm.201702116)

Senanayake, R. D., A. J. Neukirch, E. Guidez, O. V. Prezhdo and C. M. Aikens. Theoretical Investigation of Relaxation Dynamics in Au (SH) Thiolate-Protected Gold Nanoclusters. 2018. *The Journal of Physical Chemistry C*. **122** (28): 16380-16388. (LA-UR-18-22220 DOI: 10.1021/acs.jpcc.8b03595)

*Shrestha, S., H. Tsai, M. D. Yoho, D. Ghosh, Y. Lei, F. Liu, J. K. S. Baldwin, S. Xu, S. Tretiak, D. T. Vo and W. Nie. Role of the Metal–Semiconductor Interface in Halide Perovskite Devices for Radiation Photon Counting. 2020. *Nano Letters*. acsami.0c11805. (LA-UR-20-21817 DOI: 10.1021/acsami.0c11805)

*M. Soe, C. M., C. C. Stoumpos, M. Kepenekian, B. Traor \xc3\xa9, H. Tsai, W. Nie, B. Wang, C. Katan, R. Seshadri, A. D. Mohite, J. Even, T. J. Marks and M. G. Kanatzidis. New Type of 2D Perovskites with Alternating Cations in the Interlayer Space, (C(NH))(CH NH) Pb I : Structure, Properties, and Photovoltaic Performance. 2017. *Journal of the American Chemical Society*. **139** (45): 16297-16309. (LA-UR-18-30095 DOI: 10.1021/jacs.7b09096)

*M. Soe, C. M., G. P. Nagabhushana, R. Shivaramaiah, H. Tsai, W. Nie, J. Blancon, F. Melkonyan, D. H. Cao, B. Traore, L. Pedesseau, M. Kepenekian, C. Katan, J. Even, T. J. Marks, A. Navrotsky, A. D. Mohite, C. C. Stoumpos and M. G. Kanatzidis. Homologous 2D Halide Perovskites: How Thick Can They Get?. 2019. *Proceedings of the National Academy of Sciences*. **116** (1): 58-66. (LA-UR-19-20438 DOI: 10.1073/pnas.1811006115)

*M. Soe, C. M., W. Nie, C. C. Stoumpos, H. Tsai, J. Blancon, F. Liu, J. Even, T. J. Marks, A. D. Mohite and M. G. Kanatzidis. Understanding Film Formation Morphology and Orientation in High Member 2D Ruddlesden-Popper Perovskites for High-Efficiency Solar Cells. 2018. *Advanced Energy Materials*. **8** (1): 1700979. (LA-UR-18-30010 DOI: 10.1002/aenm.201700979)

*Tisdale, J. T., M. Yoho, H. Tsai, S. Shrestha, K. Fernando, J. K. Baldwin, S. Tretiak, V. Duc and W. Nie. Methylammonium Lead Tribromide Single Crystal Detectors towards Robust Gamma-Ray Photon Sensing. 2020. *Advanced Optical Materials*. **8** (10): 2000233. (LA-UR-20-20127 DOI: 10.1002/adom.202000233)

*Traore, B., L. Pedesseau, L. Assam, X. Che, J. Blancon, H. Tsai, W. Nie, C. C. Stoumpos, M. G. Kanatzidis, S. Tretiak, A. D. Mohite, J. Even, M. Kepenekian and C. Katan. Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. 2018. *ACS Nano*. **12** (4): 3321-3332. (LA-UR-18-20159 DOI: 10.1021/acsnano.7b08202)

Tretiak, S., B. Traor\xc3\xa9, L. Pedesseau, J. C. Blancon, A. D. Mohite, J. Even, C. Katan and M. Kepenekian. Critical role of vacancies and doping in nickel oxidebased halide perovskite solar cells. Submitted to *ACS Nano*. (LA-UR-19-25231)

Tretiak, S., B. Traor\xc3\xa9, L. Pedesseau, J. R. Blancon, A. D. Mohite, J. Even, C. Katan and M. Kepenekian. Critical role of vacancies and doping in nickel oxide based halide perovskite solar cells. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-20-21413)

*Tsai, H., C. Liu, E. Kinigstein, M. Li, S. Tretiak, M. Cotlet, X. Ma, X. Zhang and W. Nie. Critical Role of Organic Spacers for Bright 2D Layered Perovskites Light-Emitting Diodes. 2020. *Advanced Science*. **7** (7): 1903202. (LA-UR-19-20440 DOI: 10.1002/advs.201903202)

*Tsai, H., C. Liu, E. Kinigstein, M. Li, S. Tretiak, M. Cotlet, X. Ma, X. Zhang and W. Nie. Critical Role of Organic Spacers for Bright 2D Layered Perovskites Light-Emitting Diodes. 2020. *Advanced Science*. **7** (7): 1903202. (LA-UR-19-25919 DOI: 10.1002/advs.201903202)

Tsai, H., D. Ghosh, E. Kinigstein, B. Dryzhakov, H. R. Driscoll, M. T. Owczarek, B. Hu, X. Zhang, S. Tretiak and W. Nie. Light Induced Structural Dynamics and the Charge Transport in Butylamine Lead Bromide Layered Perovskite Thin Films. Submitted to *Nature Materials*. (LA-UR-21-31869)

*Tsai, H., F. Liu, K. Fernando, B. L. Scott, S. Tretiak, D. T. Vo, J. Strzalka and W. Nie. A sensitive and robust thin-film x-ray detector using 2D layered perovskite diodes. 2020. *Nature*. **6** (15): eaay0815. (LA-UR-19-22971 DOI: 10.1126/sciadv.aay0815)

*Tsai, H., R. Asadpour, J. Blancon, C. C. Stoumpos, J. Even, P. M. Ajayan, M. G. Kanatzidis, M. A. Alam, A. D. Mohite and W. Nie. Design principles for electronic charge transport in solution-processed vertically stacked 2D perovskite quantum wells. 2018. *Nature Communications*. **9** (1): 2130. (LA-UR-18-30079 DOI: 10.1038/s41467-018-04430-2)

Tsai, H., R. Asadpour, J. R. Blancon, C. C. Stoumpos, O. Durand, J. Strzalka, B. Chen, R. Verduzco, P. M. Ajayan, S. Tretiak, J. Even, M. A. Alam, M. G. Kanatzidis, W. Nie and A. Mohite. Light-induced lattice expansion leads to high-efficiency perovskite solar cells. Submitted to *Science*. (LA-UR-18-30082)

Tsai, H., W. Huang, R. Vil\xc3\xa1, C. Liu, X. Wen, m. Li, G. Wiederrecht, M. Cotlet, Y. Cui, Z. Zhang, X. Ma and W. Nie. Perovskite Nanocrystals Stabilized in Metal-Organic Frameworks for Bright Light Emitting Diodes. Submitted to *Nature Nanotechnology*. (LA-UR-20-23017)

Tsai, H., W. Nie and A. Mohite. Response to Comment on "Light-induced lattice expansion leads to high-efficiency solar cells". Submitted to *Science*. (LA-UR-21-22544)

*B. T. *. W. B. *. T. S. *. Z. L. Yan, L. *. and S. Tretiak. Single-Layer Dititanium Oxide Ti2O MOene: Multifunctional Promises for Electride, Anode Materials, and Superconductor. 2021. *The Journal of Physical Chemistry Letters*. **12** (1): 494-500. (LA-UR-20-24347 DOI: 10.1021/acs.jpclett.0c03397)

*Zhang, F., J. F. Castaneda, S. Chen, W. Wu, M. J. DiNezza, M. Lassise, W. Nieg, A. Mohite, Y. Liu, S. Liu, D. Friedman, H. Liu, Q. Chen, Y. Zhang, J. Huang and Y. Zhang. Comparative studies of optoelectrical properties of prominent PV materials: Halide perovskite, CdTe, and GaAs. 2020. *Materials Today*. **36**: 18-29. (LA-UR-19-28480 DOI: 10.1016/j.mattod.2020.01.001)

Zhou, L., A. J. Neukirch, D. J. Vogel, D. S. Kilin, L. Pedesseau, M. Carignano, A. Mohite, J. Even, C. Katan and S. Tretiak. Denisty of States Broadening in Ch3NH3PbI3 Hybrid Perovskites Understood from ab initio Molecular Dynamics Simulations. Submitted to *ACS Energy Letters*. (LA-UR-19-20078)

Zhou, L., C. Katan, W. Nie, H. Tsai, L. Pedesseau, J. J. Crochet, J. Even, A. Mohite, S. Tretiak and A. J. Neukirch. Cation Alloying Destabilizes Polarons in Lead-halide Perovskites. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-20075)

*Zhou, L., Y. Zhang, Z. Zhuo, A. J. Neukirch and S. Tretiak. Interlayer-Decoupled Sc-Based Mxene with High Carrier Mobility and Strong Light-Harvesting Ability. 2018. *The Journal of Physical Chemistry Letters*. **9** (23): 6915-6920. (LA-UR-18-25396 DOI: 10.1021/acs.jpclett.8b03077)

Zhou, Y., K. Fernando, J. Wan, F. Liu, S. Shrestha, J. T. Tisdale, H. Tsai, S. Tretiak, H. Huang and W. Nie. Millimeter-size all-inorganic perovskite crystalline thin film grown by chemical vapor deposition. Submitted to *Advanced Functional Materials*. (LA-UR-21-20964)

Books/Chapters

Tsai, H., J. T. Tisdale, S. Shrestha, F. Liu and W. Nie. Emerging lead-halide perovskite semiconductor for solid-state detectors. (LA-UR-20-25807)

Reports

Leak, C. O. and S. F. Nowicki. Backplane and Mounting Board for Testing Perovskite Radiation Sensors. Unpublished report. (LA-UR-19-27971)

Neukirch, A. J. Rational Design of Halide Perovskites for Next Generation Gamma-ray Detection. Unpublished report. (LA-UR-20-26868)

Neukirch, A. J. Computational Modeling for the Development of Chiral Quantum Systems. Unpublished report. (LA-UR-20-27856)

Neukirch, A. J. LDRD Data Sheet for Project 20210672ECR. Unpublished report. (LA-UR-20-29909)

Neukirch, A. J. RATIONAL DESIGN OF HALIDE PEROVSKITES FOR NEXT GENERATION GAMMA-RAY DETECTION. Unpublished report. (LA-UR-21-24319)

Neukirch, A. J., S. Tretiak and D. Ghosh. Rational Design of Halide Perovskite for Next Generation Gamma-ray detection. Unpublished report. (LA-UR-19-28486)

Neukirch, A. J. and A. Piryatinski. Layered halide perovskites as new materials for nano-structured photocathodes. Unpublished report. (LA-UR-17-30839)

Neukirch, A. J. and C. A. Mora Perez. Outline paper-v3. Unpublished report. (LA-UR-20-25928)

Neukirch, A. J. and S. Tretiak. Computational Modeling of Solid-State Detectors. Unpublished report. (LA-UR-18-24306)

Neukirch, A. J. and Y. Wang. Nonadiabatic molecular dynamics analysis of hybrid Dion-Jacobson 2D lead Iodide perovskites. Unpublished report. (LA-UR-20-25929)

Presentation Slides

Blancon, J. R. Optoelectronic properties of hybrid perovskite quantum wells. Presented at *ESP Santa Fe 2018*, Santa Fe, New Mexico, United States, 2018-06-03 - 2018-06-07. (LA-UR-18-24802)

Blancon, J. R. Exciton properties in Ruddlesden-Popper 2D Perovskites. Presented at *MRS spring 2018*, Phoenix, Arizona, United States, 2018-04-02 - 2018-04-06. (LA-UR-18-22824)

Blancon, J. R. Extremely Efficient Internal Exciton Dissociation through Edge-States in Layered 2D Perovskites for High-Efficiency Optoelectronic Devices. Presented at *MRS Spring 2018*, Phoenix, Arizona, United States, 2018-04-02 - 2018-04-06. (LA-UR-18-22826)

Blancon, J. R., H. Tsai, W. Nie, A. V. Stier, C. Stoumpos, M. Kepenekian, S. Tretiak, C. Katan, M. Kanatzidis, S. A. Crooker, J. Even, J. J. Crochet and A. Mohite. Extremely Efficient Internal Exciton Dissociation through Edge-States in Layered 2D Perovskites for High-Efficiency Optoelectronic Devices. Presented at *MRS Fall 2017*, Boston, Massachusetts, United States, 2017-11-27 - 2017-12-01. (LA-UR-17-30703)

Leveillee, J. A., A. J. Neukirch, A. Schleife and S. Tretiak. Electronic structure and optical response of layered hybrid perovskites with single \xcf\x80-conjugated organic layers.

Presented at *APS March Meeting*, Los Angeles, California, United States, 2018-03-03 - 2018-03-09. (LA-UR-18-21688)

Leveillee, J. A., A. J. Neukirch and S. Tretiak. Predicting organic layer candidates for triplet-augmented emission in layered hybrid organic-inorganic perovskite LEDs. . (LA-UR-18-27035)

Lewis, S. G., A. J. Neukirch and S. Tretiak. Investigating the Effect of Cesium Coatings on the Work Function of Cesium Lead Halide Perovskites. . (LA-UR-18-27062)

Liu, F. Graphene, TMD and heterojunction/crystals. Presented at *UESTC International Forum for Young Scholars*, Chengdu, China, 2018-11-22 - 2018-11-23. (LA-UR-18-30130)

Liu, F. Heterostructures Based on 2D Materials. . (LA-UR-19-31053)

Mohite, A. Hybrid perovskites: An ideal materials platform with emergent functional properties. Presented at *LIGHT MANAGEMENT IN PHOTOVOLTAICS*, AMSTERDAM, Netherlands, 2018-06-15 - 2018-06-15. (LA-UR-18-25142)

Neukirch, A. J. Polarons and Excitons in 2D and 3D Halide Perovskites. Presented at *Electronic and structural dynamics in hybrid perovskites: theory meets experiment*, Telluride, Colorado, United States, 2018-07-17 - 2018-07-21. (LA-UR-18-26614)

Neukirch, A. J. Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Replacement in Halide Perovskites. Presented at *NanoGe*, Malaga, Spain, 2018-10-22 - 2018-10-22. (LA-UR-18-30022)

Neukirch, A. J. Catching the Sun and Beyond: The development of perovskites for efficient photovoltaic and detector applications. Presented at *Telluride Summer Lecture Series*, Telluride, Colorado, United States, 2020-07-16 - 2020-07-16. (LA-UR-20-25251)

Neukirch, A. J. Catching the Sun and Beyond: The development of perovskites for efficient photovoltaic and detector applications. . (LA-UR-21-21882)

Neukirch, A. J. RATIONAL DESIGN OF HALIDE PEROVSKITES FOR NEXT GENERATION GAMMA-RAY DETECTION. . (LA-UR-21-24320)

Neukirch, A. J., D. Ghosh and S. Tretiak. The effect on the optoelectronic properties and charge carrier dynamics in halide perovskites due to lattice expansion. Presented at *APS March Meeting*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22469)

Neukirch, A. J., S. G. Lewis, D. Ghosh, K. L. Jensen, F. Liu, W. Nie, N. A. Moody, A. Mohite and S. Tretiak. Tuning halide perovskite work functions with Cs coatings for photocathode applications. Presented at *American Chemical Society*, Orlando, Florida, United States, 2019-04-01 - 2019-04-01. (LA-UR-19-22943)

Neukirch, A. J., S. Tretiak, L. Zhou, J. Even and I. Abate. Geometry Distortion and Small Polaron Binding Energy changes with Ionic Substitution in Halide Perovskites.

Presented at *APS March Meeting*, Los Angelos, California, United States, 2018-03-05 - 2018-03-09. (LA-UR-18-21692)

Neukirch, A. J. and A. Forde. Chiroptical Properties Induced into a Lead-Halide Perovskite Cluster Through Surface Chemistry. . (LA-UR-20-28547)

Neukirch, A. J. and S. Tretiak. Shining light on excited-state dynamics in perovskite material. . (LA-UR-18-25905)

Neukirch, A. J. and S. Tretiak. w18_gammaray_viewgraph. . (LA-UR-19-21989)

Nie, W. Perovskite Semiconductors for Opto-Electronic Device and Radiation Detector. . (LA-UR-19-28791)

Nie, W. Hybrid perovskite semiconductors for solid state radiation detectors. Presented at *47th Conference on the Physics and Chemistry of Surfaces and Interfaces*, boulder, Colorado, United States, 2020-01-19 - 2020-01-23. (LA-UR-20-20342)

Nie, W. 2D perovskite optoelectronic device physics. Presented at *Perovskite Material Webinar*, Los Alamos, New Mexico, United States, 2020-05-21 - 2020-05-31. (LA-UR-20-23709)

Nie, W. Metal Halide Hybrid Perovskite Semiconductors for Opto-Electronic Device. . (LA-UR-20-27014)

Nie, W. 3D and 2D Perovskite Semiconductors for Photovoltaics. Presented at *Web Seminar at First Solar*, San Jose, California, United States, 2020-10-14 - 2020-10-14. (LA-UR-20-28043)

Nowicki, S. F., C. O. Leak, J. T. Tisdale, D. T. Vo and M. D. Yoho. Performance Characterization of Halide Perovskite Detectors. . (LA-UR-20-21314)

Shrestha, S. The Role of Metal-Semiconductor Interface in Hybrid Perovskite Devices for High-Performance Solid-State Detector. Presented at *Material Research Society, boston*, boston, Michigan, United States, 2019-12-02 - 2019-12-08. (LA-UR-19-32154)

Shrestha, S., H. Tsai, F. Liu, M. D. Yoho, J. K. S. Baldwin, S. Tretiak, D. T. Vo, Y. Lei, S. Xu and W. Nie. The Role of Metal-Semiconductor Interface in Hybrid Perovskite Devices for High-Performance Solid-State Detector. Presented at *MRS Boston*, Boston, Massachusetts, United States, 2019-12-01 - 2019-12-01. (LA-UR-19-31945)

Smith, B. A., L. Zhou, A. J. Neukirch, S. Tretiak and A. V. Akimov. Non-Adiabatic Molecular Dynamics with Spin-Orbit Coupling. . (LA-UR-18-28269)

Smith, B. A., L. Zhou, A. J. Neukirch, S. Tretiak and A. V. Akimov. UPDATE 8/13/18. . (LA-UR-18-28262)

Tisdale, J. T. and W. Nie. Robust Perovskite Single Crystal Devices for Efficient Gamma-Ray Detection. Presented at *Material Research Society*, boston, Michigan, United States, 2019-12-02 - 2019-12-08. (LA-UR-19-32314)

Tretiak, S. Rational design of halide perovskites for next generation Gamma-ray detection. . (LA-UR-19-20464)

Tretiak, S. Modeling of Electronic Properties in Organic and Hybrid Materials. . (LA-UR-19-28826)

Tretiak, S. Rational design of halide perovskites for next generation Gamma-ray detection (3rd year review, talks). . (LA-UR-20-21096)

Tretiak, S. "Rational design of halide perovskites for next generation Gamma-ray detection (3rd year review, posters)". . (LA-UR-20-21097)

Tretiak, S. Hybrid 2D and 3D Nanostructured Perovskites: From Understanding Fundamental Physics to Optoelectronic Applications. Presented at *Virtual International Workshop on Nanotechnology*, Tbilisi, Georgia, 2020-10-05 - 2020-10-05. (LA-UR-20-27741)

Zhou, L. Polaron Behaviors in Hybrid Lead-halide Perovskites. Presented at *Spring 2019 National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22860)

Posters

Fernando, K., F. Liu, S. Shrestha, J. Wan, H. Tsai and W. Nie. The physical origin of defect and transport for perovskite single crystal. Presented at *2019 UNM STEM research symposium*, Alburquerque, New Mexico, United States, 2019-03-02 - 2019-03-02. (LA-UR-19-21949)

Leak, C. O., S. F. Nowicki, J. T. Tisdale, R. C. Schirato, C. D. Roecker and J. F. Dowd. Performance Characterization of Halide Perovskites for Hard-Radiation Spectroscopy. Presented at *IEEE Nuclear Science Symposium*, Manchester, United Kingdom, 2019-10-26 - 2019-10-26. (LA-UR-19-31026)

Leveillee, J. A. and A. Schleife. Free-carrier and polar lattice screening of excitons in hybrid perovskite MAPbI3. Presented at *Excited State Processes Conference*, Santa Fe, New Mexico, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-24685)

Lewis, S. G., D. Ghosh, A. J. Neukirch and S. Tretiak. Surface Core-Level Shifts of Lead Halide Perovskites. . (LA-UR-19-27762)

Lewis, S. G. and A. J. Neukirch. Tuning the work function of organometallic halide perovskites with Cs. Presented at *Excited State Processes in Electronic and Bio Nanomaterials (ESP-2018)*, Santa Fe, New Mexico, United States, 2018-06-04 - 2018-06-08. (LA-UR-18-24630)

Neukirch, A. J., C. A. Mora Perez, D. Ghosh, S. Tretiak and O. Prezhdo. TDDFT Characterization of a CsPbBr3 Clusters' Optical Properties. Presented at *TDDFT Workshop*, Newark, New Jersey, United States, 2019-08-05 - 2019-08-09. (LA-UR-19-27716)

Neukirch, A. J., S. G. Lewis, D. Ghosh and S. Tretiak. Surface Core-Level Shifts of Lead Halide Perovskites. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27718)

Neukirch, A. J., Y. Wang, D. Ghosh, S. Tretiak and O. Prezhdo. Electron-Hole recombination of Hybrid Dion-Jacobson 2D Lead Iodide Perovskites: Nonadiabaitc Molecular Dynamics Analysis. Presented at *TDDFT Workshop*, Newark, New Jersey, United States, 2019-08-05 - 2019-08-09. (LA-UR-19-27717)

Shrestha, S., H. Tsai, F. Liu, J. T. Tisdale, Y. Lei, M. D. Yoho, J. K. S. Baldwin, S. Tretiak, D. T. Vo and W. Nie. The Role of Metal-Semiconductor Interface in Hybrid Perovskite Devices for High-Performance Solid-State Detector. Presented at *LANL Postdoc Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28647)

Tisdale, J. T., M. D. Yoho, C. O. Leak, S. Shrestha, H. Tsai, C. D. Roecker, S. F. Nowicki, D. T. Vo, S. Tretiak and W. Nie. Novel Hybrid Perovskite Semiconductors towards Low-Cost, Room Temperature Gamma Spectroscopy. Presented at *LANL Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28606)

Tsai, H., F. Liu, S. Shrestha, K. Fernando, S. Tretiak, B. L. Scott, D. T. Vo, J. Strzalka and W. Nie. Highly Sensitive, Self-powered Thin Film X-ray Detector Using Ruddlesden-Popper Phase Layered Perovskite Diodes. Presented at *LANL Post-Doc Research Day*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28484)

Driven Quantum Matter: A Route Towards Novel Phases

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20190026DR

Project Description

The discovery of new materials has played a significant part in nearly every technological leap forward. To date, these advances have relied on conventional materials, which are now reaching their intrinsic limits. Quantum materials can enable us to overcome this, as they offer a host of unique properties that could be the basis of the next technological revolution, impacting areas including quantum computing and energy-efficient sensing. However, it has been difficult to tailor them for such applications, likely because conventional equilibrium tuning methods (e.g., temperature and pressure) make it difficult to realize a desired state of matter. Intense, transient electromagnetic (EM) fields have recently emerged as an exciting alternative for driving quantum materials into new states. However, these states have thus far been discovered by chance, making it vital to develop new approaches for predicting and controlling EM-driven phases. The objective of this project is to move beyond serendipitous discovery to demonstrate a world-leading capability for predicting and realizing novel EM-driven quantum phases, accomplished by pursuing an integrated theoretical and experimental approach focusing on three representative classes of quantum materials. This will impact a wide range of mission-relevant objectives, including novel materials for energy-efficient sensing, data storage, and computation.

Technical Outcomes

The project successfully achieved the goal of developing and applying advanced theoretical methods to predict novel states in driven quantum materials, one of the most important Los Alamos materials strategies. The new theoretical capabilities have also cemented the connection with one of the leading ultrafast optical laboratories and one of the leading pulsed magnetic field facilities in the world. It attracted young talent, which is essential for the future sustainability of the workforce.

Publications

Journal Articles

Ahmed, T., R. P. Prasankumar, J. Yoo and J. Zhu. A real-time TDDFT study of femtosecond laser driven monolayer NbSe2. Submitted to *Physical Review B*. (LA-UR-20-26231)

*Asaba, T., Y. Su, M. Janoschek, J. D. Thompson, S. M. Thomas, E. D. Bauer, S. Lin and F. Ronning. Large tunable anomalous Hall effect in the kagome antiferromagnet U3Ru4Al12. 2020. *Nature Communications*. **102** (3): 35127. (LA-UR-19-25889 DOI: 10.1103/PhysRevB.102.035127)

Banerjee, S., U. Kumar and S. Lin. Inverse Faraday effect in Mott insulators. Submitted to *Physical Review Letters*. (LA-UR-21-28801)

Bonca, J., S. A. Trugman and M. Berciu. Spectral Function of the Holstein Polaron at Finite Temperature. Submitted to *Physical Review B*. (LA-UR-20-21134)

Bonca, J. and S. A. Trugman. Dynamic properties of a polaron coupled to dispersive optical phonons. Submitted to *Physical Review B*. (LA-UR-20-30004)

Cao, C. and J. Zhu. Pressure Dependent Electronic Structure in CeRh6Ge4. Submitted to *Physical Review Letters*. (LA-UR-20-29736)

*Chen, A., Q. Su, H. Han, E. Enriquez and Q. Jia. Metal Oxide Nanocomposites: A Perspective from Strain, Defect, and Interface. 2019. *Advanced Materials*. **31** (4): 1803241. (LA-UR-19-29397 DOI: 10.1002/adma.201803241)

*Chen, A., W. Zhang, L. R. Dedon, D. Chen, F. Khatkhatay, J. L. MacManus-Driscoll, H. Wang, D. A. Yarotski, J. Chen, X. Gao, L. W. Martin, A. Roelofs and Q. Jia. Couplings of Polarization with Interfacial Deep Trap and Schottky Interface Controlled Ferroelectric Memristive Switching. 2020. *Advanced Functional Materials*. **30** (43): 2000664. (LA-UR-20-26857 DOI: 10.1002/adfm.202000664)

*Chen, A., Y. Dai, A. Eshghinejad, Z. Liu, Z. Wang, J. Bowlan, E. Knall, L. Civale, J. L. MacManus-Driscoll, A. J. Taylor, R. P. Prasankumar, T. Lookman, J. Li, D. Yarotski and Q. Jia. Competing Interface and Bulk Effect–Driven Magnetoelectric Coupling in Vertically Aligned Nanocomposites. 2019. *Advanced Science*. **6** (19): 1901000. (LA-UR-19-27192 DOI: 10.1002/advs.201901000)

*Chen, A., Z. Harrell, P. Lu, E. Enriquez, L. Li, B. Zhang, P. Dowden, C. Chen, H. Wang, J. L. MacManus-Driscoll and

Q. Jia. Strain Enhanced Functionality in a Bottom-Up Approach Enabled 3D Super-Nanocomposites. 2019. *Advanced Functional Materials*. **29** (26): 1900442. (LA-UR-19-29645 DOI: 10.1002/adfm.201900442)

*Chen, A. and Q. Jia. A pathway to desired functionalities in vertically aligned nanocomposites and related architectures. 2021. *MRS Bulletin*. **46** (2): 115-122. (LA-UR-21-21607 DOI: 10.1557/s43577-021-00032-4)

*Chen-Yen, L. and Z. Jian-Xin. Ultrafast X-Ray Absorption Spectroscopy of Strongly Correlated Systems: Core Hole Effect. 2019. *Physical Review Letters*. **122** (20): 207401. (LA-UR-17-29749 DOI: 10.1103/PhysRevLett.122.207401)

*Cheng, L., T. Sarkar, J. Lourembam, R. Tutchton, M. Motapathula, D. Zhao, J. Zhu, T. Venkatesan and E. E. M. Chia. Observation of interacting polaronic gas behavior in Ta-doped TiO_2 thin films via terahertz time-domain spectroscopy. 2020. *Applied Physics Letters*. **117** (26): 261902. (LA-UR-20-29910 DOI: 10.1063/5.0022775)

Corey, Z. J., H. Han, K. T. Kang, X. Wang, B. Paudel, P. Roy, Y. Sharma, J. Yoo, Q. Jia and A. Chen. Origin of the enhanced conductivity in $La_{0.95}Sr_{0.05}TiO_3/SrTiO_3$ heterostructures. Submitted to *Advanced Materials Interfaces*. (LA-UR-21-30173)

*Ding, X., B. Gao, E. Krenkel, C. Dawson, J. C. Eckert, S. Cheong and V. Zapf. Magnetic properties of double perovskite Ln_2CoIrO_6 (Ln=Eu, Tb, Ho): Hetero-tri-spin 3d–5d–4f systems. 2019. *Physical Review B*. **99** (1): 14438. (LA-UR-18-30816 DOI: 10.1103/PhysRevB.99.014438)

*Dong, W., D. Cortie, T. Lu, Q. Sun, N. Narayanan, W. Hu, L. Jacob, Q. Li, D. Yu, H. Chen, A. Chen, X. Wei, G. Wang, M. G. Humphrey, T. J. Frankcombe and Y. Liu. Collective nonlinear electric polarization via defect-driven local symmetry breaking. 2019. *Materials Horizons*. **6** (8): 1717-1725. (LA-UR-21-22624 DOI: 10.1039/C9MH00516A)

*Duan, C., K. Sasmal, M. B. Maple, A. Podlesnyak, J. Zhu, Q. Si and P. Dai. Incommensurate Spin Fluctuations in the Spin-triplet Superconductor Candidate UTe_2. 2020. *Physical Review Letters*. **125** (23): 237003. (LA-UR-20-24870 DOI: 10.1103/PhysRevLett.125.237003)

*Enriquez, E. M., Q. Li, P. R. Bowlan, P. Lu, B. Zhang, L. Li, H. Wang, A. J. Taylor, D. A. Yarotski, R. P. Prasankumar, S. V. Kalinin, Q. Jia and A. Chen. Induced ferroelectric phases in $SrTiO$ by a nanocomposite approach. 2020. *Nanoscale*. **12** (35): 18193-18199. (LA-UR-20-24150 DOI: 10.1039/D0NR03460F)

*Fauseweh, B. and J. Zhu. Laser pulse driven control of charge and spin order in the two-dimensional Kondo lattice. 2020. *Physical Review B*. **102** (16): 165128. (LA-UR-20-21229 DOI: 10.1103/PhysRevB.102.165128)

Fauseweh, B. and J. Zhu. Digital Quantum Simulation of Non-Equilibrium Quantum Many-Body Systems. Submitted to *Nature*. (LA-UR-20-27234)

Fauseweh, B. and J. Zhu. Digital Quantum Simulation of Non-Equilibrium Quantum Many-Body Systems. Submitted to *Quantum Information Processing*. (LA-UR-21-21981)

Fauseweh, B. and J. Zhu. Ultrafast Optical Control of Magnetic Order and Fermi Surface Topology at a Quantum Critical Point. Submitted to *Science Advances*. (LA-UR-21-25611)

Ferkinghoff, G., M. Leanna, U. Goetz, U. Kumar and B. Fauseweh. Accessing Multi-triplons in Spin Ladders using Resonant Inelastic X-ray Scattering. Submitted to *Physical Review Letters*. (LA-UR-20-29911)

Geihufe, R. M., V. Juricic, S. Bonetti, J. Zhu and A. V. Balatsky. Dynamically induced magnetism in $KaTaO_3$. Submitted to *Physical Review Research*. (LA-UR-21-22203)

*Gupta, S. and A. Saxena. Curvature distribution and autocorrelations in elliptic cylinders and cones. 2019. *AIP Advances*. **9** (8): 085304. (LA-UR-19-23839 DOI: 10.1063/1.5106380)

*Hesler, J., R. Prasankumar and J. Tignon. Advances in terahertz solid-state physics and devices. 2019. *Journal of Applied Physics*. **126** (11): 110401. (LA-UR-19-29705 DOI: 10.1063/1.5122975)

Huang, J., R. Yu, Z. Xu, J. Zhu, Q. Jiang, M. Wang, H. Wu, T. Chen, J. Denlinger, S. Mo, M. Hashimoto, G. Gu, P. Dai, J. Chu, D. H. Lu, Q. Si, R. Birgeneau and M. Yi. Low Temperature Emergence of an Orbital-Selective Mott Phase in $FeTe_{1-x}Se_x$. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-27137)

Huang, Z., C. S. Ting, J. Zhu and S. Lin. Gapless Higgs Mode in the Fulde-Ferrell-Larkin-Ovchinnikov State of a Superconductor. Submitted to *Physical Review Letters*. (LA-UR-21-24876)

*Khare, A. and A. Saxena. Family of potentials with power law kink tails. 2019. *Journal of Physics A: Mathematical and Theoretical*. **52** (36): 365401. (LA-UR-18-30274 DOI: 10.1088/1751-8121/ab30fd)

*Kim, J., X. Wang, F. Huang, Y. Wang, X. Fang, X. Luo, Y. Li, M. Wu, S. Mori, D. Kwok, E. D. Mun, V. S. Zapf and S. Cheong. Spin Liquid State and Topological Structural Defects in Hexagonal. 2019. *Physical Review X*. **9** (3): 031005. (LA-UR-18-30066 DOI: 10.1103/PhysRevX.9.031005)

Kumar, U., A. Nag, J. Li, H. C. Robarts, A. C. Walters, M. Garcia-Fernandez, R. Saint-Martin, A. Revcolevschi, J. Schlappa, T. Schmitt, S. Johnston, K. Zhou and S. Banerjee. Unraveling higher-order corrections in the spin dynamics of RIXS spectra. Submitted to *Physical Review Letters*. (LA-UR-21-29415)

Kumar, U. and S. Lin. Inducing and controlling superconductivity in Hubbard honeycomb model using an electromagnetic drive. Submitted to *Physical Review B*. (LA-UR-20-30127)

Lai, C. Y. and S. A. Trugman. Absence of diffusion and fractal geometry in the Holstein model at high temperature. Submitted to *Physical Review Letters*. (LA-UR-20-24815)

Li, H., U. Kumar, K. Sun and S. Lin. Spontaneous fractional Chern insulators in transition metal dichacogenides Moir\xc3\xa9 superlattices. Submitted to *Physical Review Letters*. (LA-UR-21-20020)

Li, L., J. Cheng, H. Wang, J. Huang, X. Gao, X. Wang, S. Misra, B. Zhang, J. Jian, A. Chen, P. Lu, X. Qian, K. Yang and H. Wang. Interfacial Engineering Enabled Novel Bi-Based Layered Oxide Supercells with Modulated Microstructures and Tunable Physical Properties. Submitted to *Crystal Growth & Design*. (LA-UR-20-24154)

Li, S., A. Nocera, U. Kumar and S. Johnston. Particle-hole asymmetry in the dynamical spin and charge structure factors of the corner-shared one-dimensional cuprates. Submitted to *Nature Communications*. (LA-UR-21-23606)

*Li, W., B. Zhu, R. Zhu, Q. Wang, P. Lu, Y. Sun, C. Cafolla, Z. Qi, A. Chen, P. Gao, H. Wang, Q. He, K. Zhang and J. L. MacManus-Driscoll. Atomic-Scale Control of Electronic Structure and Ferromagnetic Insulating State in Perovskite Oxide Superlattices by Long-Range Tuning of BO Octahedra. 2020. *Advanced Functional Materials*. **30** (40): 2001984. (LA-UR-20-28256 DOI: 10.1002/adfm.202001984)

Lin, H., R. Yu, J. Zhu and Q. Si. Orbital-selective correlations and renormalized electronic structure in LiFeAs. Submitted to *Physical Review Letters*. (LA-UR-21-20306)

*Liu, J., L. Cheng, D. Zhao, X. Chen, H. Sun, J. Zhu, Z. Li, X. Wang and E. E. M. Chia. Quenching of the relaxation pathway in the Weyl semimetal TaAs. 2020. *Physical Review B*. **102** (6): 064307. (LA-UR-20-21231 DOI: 10.1103/PhysRevB.102.064307)

*Lu, X., A. Chen, Y. Dai, B. Wei, H. Xu, J. Wen, N. Li, Y. Luo, X. Gao, E. Enriquez, Z. Wang, P. Dowden, W. Yang, Y. Zhao and Q. Jia. Metallic interface induced by electronic reconstruction in crystalline-amorphous bilayer oxide films. 2019. *Science Bulletin*. **64** (21): 1567-1572. (LA-UR-19-29647 DOI: 10.1016/j.scib.2019.08.026)

*Mbatang, R., D. Xue, E. Enriquez, R. Yuan, H. Han, P. Dowden, Q. Wang, E. Fohtung, D. Xue, T. Lookman, S. J. Pennycook and A. Chen. Enhanced magnetism in lightly doped manganite heterostructures: strain or stoichiometry?. 2019. *Nanoscale*. **11** (15): 7364-7370. (LA-UR-19-25634 DOI: 10.1039/C8NR09693G)

*Merkli, M., G. P. Berman and A. Saxena. Quantum electron transport in degenerate donor–acceptor systems. 2020. *Journal of Mathematical Physics*. **61** (7): 072102. (LA-UR-19-31360 DOI: 10.1063/1.5138725)

Nekreshevich, I., X. Ding, F. F. Balakirev, H. T. Yee, S. W. Cheong, L. Civale, Y. Kamiya and V. Zapf. Reaching the equilibrium state of frustrated triangular Ising magnet Ca3Co2O6. Submitted to *Physical Review B*. (LA-UR-22-20369)

Padmanabhan, P., F. L. Buessen, R. M. Tutchton, K. W. C. Kwock, S. D. Gilinsky, M. C. Lee, M. A. McGuire, S. R. Singamaneni, D. A. Yarotski, A. Paramekanti, J. Zhu and R. P. Prasankumar. Coherent Helicity-Dependent Spin-Phonon Oscillations in the Ferromagnetic van der Waals Crystal CrI3. Submitted to *Nature Physics*. (LA-UR-20-27954)

Padmanabhan, P., S. Boubanga-Tombet, H. Fukidome, T. Otsuji and R. P. Prasankumar. A graphene-based magnetoplasmonicmetasurface for actively tunable transmission andpolarization rotation at terahertz frequencies. Submitted to *Applied Physics Letters*. (LA-UR-19-29951)

*Paeckel, S., B. Fauseweh, A. Osterkorn, T. Koehler, D. Manske and S. R. Manmana. Detecting superconductivity out of equilibrium. 2020. *Physical Review Letters*. **101** (18): 180507. (LA-UR-19-27999 DOI: 10.1103/PhysRevB.101.180507)

*Paudel, B., B. Zhang, Y. Sharma, K. T. Kang, H. Nakotte, H. Wang and A. Chen. Anisotropic domains and antiferrodistortive-transition controlled magnetization in epitaxial manganite films on vicinal SrTiO substrates. 2020. *Applied Physics Letters*. **117** (8): 081903. (LA-UR-20-28257 DOI: 10.1063/5.0016371)

Paudel, B., K. T. Kang, Y. Sharma, H. Nakotte, D. A. Yarotski and A. Chen. Symmetry mismatch controlled ferroelastic domains ordering and functional properties of manganite films on cubic miscut substrates. Submitted to *Nanoscale*. (LA-UR-21-22621)

Paudel, B., Y. Sharma, B. K. Derby, G. Pilania, M. M. Schneider, A. C. Jones, H. Nakotte, M. T. Pettes and A. Chen. Effect of Lattice Strain on Magnetism in Epitaxial YCrO3 Films. Submitted to *APL Materials*. (LA-UR-21-24953)

*Porta, M., T. Cast\xc3\xa1n, A. Saxena and A. Planes. Influence of the number of orientational domains on avalanche criticality in ferroelastic transitions. 2019. *Physical Review E*. **100** (6): 062115. (LA-UR-19-27335 DOI: 10.1103/PhysRevE.100.062115)

Ronning, F., S. Lee, S. Seo, K. E. Avers, S. M. Thomas, R. Movshovich, J. D. Thompson, P. Rosa, E. D. Bauer and T. Asaba. Physical properties of quasi-one-dimensional YbFe5P3. Submitted to *Physical Review B*. (LA-UR-21-28341)

Saxena, A. B., K. V. Yershov, V. P. Kravchuk, D. D. Sheka and J. van den Brink. Domain wall diode based on functionally graded Dzyaloshinskii-Moriya interaction. Submitted to *Physical Review Letters*. (LA-UR-20-22584)

Saxena, A. B. and A. S. Bhalla. On Its 100th, Future Is Ferroelectric. Submitted to *Physics World*. (LA-UR-20-27846)

Saxena, A. B. and D. Schmeltzer. Superconductivity in Graphene Induced by the Rotated Layer. Submitted to *Physical Review B*. (LA-UR-20-20429)

Saxena, A. B. and D. Schmeltzer. Optical conductivity of multi-Weyl node semimetals due to electromagnetic and axial pseudogauge fields. Submitted to *Physical Review B*. (LA-UR-21-25129)

Saxena, A. B. and S. Banerjee. Higher Chern numbers in Multilayer (N >2) Lieb Lattices: Topological Transitions and Quadratic Band Crossing Lines. Submitted to *Physical Review Letters*. (LA-UR-20-25919)

*S. A. Schmeltzer, D. *. and A. Saxena. Induced axion-phason field in Weyl semimetals. 2021. *Physical Review B*. **103** (23): 235113. (LA-UR-19-31359 DOI: 10.1103/PhysRevB.103.235113)

*Schwarz, L., B. Fauseweh and D. Manske. Momentum-resolved analysis of condensate dynamic and Higgs oscillations in quenched superconductors with time-resolved ARPES. 2020. *Physical Review B*. **101** (22): 224510. (LA-UR-20-21388 DOI: 10.1103/PhysRevB.101.224510)

Sharma, Y., A. R. Mazza, B. L. Musico, E. Skoropata, R. Nepal, R. Jin, A. V. Ievlev, L. Collins, Z. Gai, A. Chen, M. Brahlek, V. Keppens and T. Z. Ward. Magnetic Texture in Insulating Single Crystal High Entropy Oxide Spinel Films. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-21-30189)

Sharma, Y., B. Paudel, J. Lee, W. S. Choi, Z. Yang, H. Wang, Y. Du, K. T. Kang, G. Pilania and A. Chen. Tuning magnetic and optical properties through strain in epitaxial LaCrO3 thin films. Submitted to *Physical Review Materials*. (LA-UR-21-20416)

Sharma, Y., B. Paudel, J. Lee, W. S. Choi, Z. Yang, H. Wang, Y. Du, K. T. Kang, G. Pilania and A. Chen. Tuning magnetic and optical properties through strain in epitaxial LaCrO3 thin films. Submitted to *Physical Review Materials*. (LA-UR-21-30199)

Sharma, Y., M. C. Lee, K. Pitike, K. K. Mishra, Q. Zheng, X. Gao, B. L. Musicao, A. R. Mazza, R. S. Katiyar, V. Keppens, M. Brahlek, D. A. Yarotski, R. P. Prasankumar, A. Chen, V. R. Cooper and T. Z. Ward. High Entropy Oxide Relaxor Ferroelectrics. Submitted to *ACS-JACS*. (LA-UR-21-24954)

*Sim, S., D. Lee, J. Lee, M. Cha, S. Cha, W. Heo, S. Cho, W. Shim, K. Lee, J. Yoo, R. P. Prasankumar, H. Choi and M. Jo. Role of weak interlayer coupling in ultrafast exciton-exciton annihilation in two-dimensional rhenium dichalcogenides. 2020. *Physical Review B*. **101** (17): 174309. (LA-UR-20-20522 DOI: 10.1103/PhysRevB.101.174309)

Su, Y., A. Masaki-Kato, W. Zhu, J. Zhu, Y. Kamiya and S. Lin. Stable Higgs mode in anisotropic quantum magnets. Submitted to *Physical Review X*. (LA-UR-20-24832)

Su, Y. and S. Lin. Topological Sliding Moire \xcc\x81 Heterostructure. Submitted to *Physical Review Letters*. (LA-UR-19-30658)

*Su, Y. and S. Lin. Current-Induced Reversal of Anomalous Hall Conductance in Twisted Bilayer Graphene. 2020. *Physical Review Letters*. **125** (22): 226401. (LA-UR-20-21206 DOI: 10.1103/PhysRevLett.125.226401)

Wang, Z., H. Zhou, M. Guo, L. Zhao, T. Xu, Y. Dong, K. Wu, S. G. Je, W. Chao, M. Im, H. Han, S. Lee, K. Lee, C. Song, H. Wu, S. Lin and W. Jiang. Thermal generation, manipulation and detection of skyrmions. Submitted to *Nature Electronics*. (LA-UR-19-25918)

Xu, C., C. Cao and J. Zhu. Pressure-induced concomitant topological and metal-insulator quantum phase transitions in Ce3Pd3Bi4. Submitted to *Nature Communications*. (LA-UR-21-28777)

*Yarmohammadi, M., C. Meyer, B. Fauseweh, B. Normand and G. S. Uhrig. Dynamical properties of a driven dissipative dimerized S=1/2 chain. 2021. *Physical Review B*. **103** (4): 045132. (LA-UR-20-27708 DOI: 10.1103/PhysRevB.103.045132)

*Ying, S., S. Hayami and L. Shi-Zeng. Dimension transcendence and anomalous charge transport in magnets with moving multiple- spin textures. 2020. *Physical Review Research*. **2** (1): 013160. (LA-UR-19-25839 DOI: 10.1103/PhysRevResearch.2.013160)

*H. H. *. N. E. M. *. Z. J. *. S. Q. Yu, R. *. and J. Zhu. Orbital Selectivity in Electron Correlations and Superconducting Pairing of Iron-Based Superconductors. 2021. *Frontiers in Physics*. **9**: 578347. (LA-UR-20-24691 DOI: 10.3389/fphy.2021.578347)

Yuan, L., J. Jeong, K. Kwock, E. Yanev, M. Grandel, D. Rhodes, T. S. Luk, J. Schuck, D. A. Yarotski, J. Hone, I. Brener and R. P. Prasankumar. Manipulation of Exciton Dynamics in Single-Layer WSe Using a Toroidal Dielectric Metasurface. 2021. *Nano Letters*. (LA-UR-21-29823 DOI: 10.1021/acs.nanolett.1c03189)

Yuan, R., P. Lu, H. Han, D. Xue, A. Chen, Q. Jia and T. Lookman. Enhanced magnetocaloric performance in manganite bilayers. Submitted to *Journal of Applied Physics*. (LA-UR-20-24153)

*G. C. *. S. L. Zhijie, F. *., F. Zhijie and L. Shi-Zeng. Enhanced superconductivity in quasiperiodic crystals. 2021. *Physical Review Research*. **3** (2): 023195. (LA-UR-20-23148 DOI: 10.1103/PhysRevResearch.3.023195)

*F. B. *. C. A. *. Z. J. Zhu, W. *., W. Zhu, B. Fauseweh, A. Chacon and J. Zhu. Ultrafast laser-driven many-body dynamics and Kondo coherence collapse. 2021. *Physical Review B*. **103** (22): 224305. (LA-UR-18-31170 DOI: 10.1103/PhysRevB.103.224305)

Books/Chapters

Saxena, A. B., P. G. Kevrekidis and J. Cuevas-Maraver. Nonlinearity and Topology. (LA-UR-19-32477)

Reports

Chen, A. High-performance Photo-sensor/detector by Multiplexed Heterojunction of 2D Epitaxial Layers/perovskites/plasmonic Nanoparticles. Unpublished report. (LA-UR-21-24666)

Chen, A. In Operando Study of Resistive-switching Devices at Nanoscale. Unpublished report. (LA-UR-21-25377)

Chen, A. High-performance Photo-sensor/detector by Multiplexed Heterojunction of 2D Epitaxial Layers/ perovskites/plasmonic Nanoparticles. Unpublished report. (LA-UR-21-25378)

Fauseweh, B. Induced Phases in Driven Strongly-Correlated Systems. Unpublished report. (LA-UR-19-28000)

Padmanabhan, P., K. W. C. Kwock, F. L. Buessen, R. M. Tutchton, S. D. Gilinsky, M. C. Lee, S. S. Rao, M. A. McGuire, D. A. Yarotski, A. Paramekanti, J. Zhu and R. P. Prasankumar. The transient properties of 2D magnets: from mechanical exfoliation to ultrafast optical spectroscopy of CrX3 materials. Unpublished report. (LA-UR-20-27568)

Saxena, A. B. and A. S. Bhalla. 100th Anniversary of the discovery of Ferroelectricity: How did it impact the Current Day Physics. Unpublished report. (LA-UR-20-24320)

Presentation Slides

Blackwell, S. B., F. B. Santos, P. Rosa, S. M. Thomas, E. D. Bauer, J. D. Thompson and F. Ronning. Studies of the Non-Centrosymmetric Superconductor ThIrSi using 29Si NMR. Presented at *APS March Meeting 2021, virtual*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22467)

Chen, A. Interplay of Strain, Defects and Interface on Functional Properties in Vertical Nanocomposites. Presented at *19th International Conference on Crystal Growth and Epitaxy (ICCGE-19)*, Keystone, Colorado, United States, 2019-07-28 - 2019-08-02. (LA-UR-19-27280)

Chen, A. Tuning functional properties in manganite heterostructures: strain or stoichiometry?. Presented at *Electronic Materials and Applications 2020*, orlando, Florida, United States, 2020-01-21 - 2020-01-21. (LA-UR-20-20799)

Chen, A. Controlling functional properties in oxide nanocomposites via strain, defects and interfaces. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-24 - 2020-02-24. (LA-UR-20-21926)

Chen, A. Correlation among strain, defect, interface and functional properties in oxide nanocomposites. Presented at *CINT user meeting*, los alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27407)

Chen, A. Manipulating Mesoscale Properties in Functional Oxide Thin Films. . (LA-UR-21-23456)

Fauseweh, B. Discovering and Detecting Dynamical Quantum Matter. Presented at *Seminar Talk PSI*, Virtual, New Mexico, United States, 2021-02-16 - 2021-02-16. (LA-UR-21-21362)

Fauseweh, B. Induced Phases in Driven Strongly-Correlated Systems. . (LA-UR-21-21949)

Fauseweh, B., W. Zhu and J. Zhu. High harmonic generation in heavy fermion systems. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22388)

Fauseweh, B. and J. Zhu. Laser pulse driven nonequilibrium dynamics in the Kondo lattice model: A TD-VMC study. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21943)

Fauseweh, B. and J. Zhu. Digital Quantum Simulation of Non-Equilibrium Quantum Many-Body Systems. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-14 - 2021-03-14. (LA-UR-21-22446)

Kumar, U. Probing and controlling quantum magnets using light. . (LA-UR-21-27197)

Kumar, U. and S. Lin. Accessing quantum phases in Hubbard honeycomb lattice using an electromagnetic drive. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21998)

Kumar, U. and S. Lin. Inducing and controlling superconductivity in Hubbard honeycomb model using an electromagnetic drive. Presented at *APS March Meeting 2021*, Nashville, Tennessee, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22430)

Lai, C. Y. Pump probe phenomena in strongly correlated systems. . (LA-UR-20-21755)

Lalk, R. A. and A. Chen. Resistive Switching in Metal/Nb:SrTiO3 Based Memristors. Presented at *Electronic Materials and Applications (EMA) 2021*, Online, New Mexico, United States, 2021-01-19 - 2021-01-22. (LA-UR-21-20021)

Lee, M., V. Zapf, D. Mandrus, J. Yan and P. Lampen-Kelley. High magnetic field study on Ir3+ doped a-RuCl3. Presented at *APS March meeting 2020 in Denver, Colorado*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21988)

Lopez-Bezanilla, A. Magnetic Monopole Kinetics in Qubit Spin Ice. Presented at *QUBITS*, Online, Canada, 2021-10-04 - 2021-10-06. (LA-UR-21-29016)

Padmanabhan, P. Uncovering ultrafast magnetic dynamics and collective excitations in quantum materials. Presented at *Seminar at Center for Functional Nanomaterials at Brookhaven National Laboratory*, Brookhaven, New York, United States, 2020-09-11 - 2020-09-11. (LA-UR-20-27097)

Padmanabhan, P., K. W. C. Kwock, L. Martinez, R. M. Tutchton, F. Buessen, S. D. Gilinsky, M. C. Lee, J. Zhu, A. Paramekanti, M. McGuire, D. A. Yarotski, S. Singamaneni and R. P. Prasankumar. Helicity-Dependent Coherent Spin-Phonon Oscillations in the Ferromagnetic van der Waals Crystal CrI3. Presented at *CLEO*, San Jose, California, United States, 2020-05-11 - 2020-05-15. (LA-UR-20-23602)

Padmanabhan, P., K. W. C. Kwock, T. Treveisan, S. D. Gilinsky, N. S. Sirica, J. Kim, P. J. Schuck, P. Orth, D. A. Yarotski, S. Cheong and R. P. Prasankumar. Large Second Harmonic Generation from Polar van der Waals Bismuth Telluro-Halide Semiconductors. Presented at *CLEO*, San Jose, California, United States, 2020-05-11 - 2020-05-15. (LA-UR-20-23642)

Padmanabhan, P. and I. Telops. Magnetoplasmonic Manipulation of THz Transmission and Faraday Rotation Using Graphene Micro-Ribbon Arrays. Presented at *CLEO*, San Jose, California, United States, 2019-05-05 - 2019-05-10. (LA-UR-19-24223)

Prasankumar, R. P. Coherent helicity-dependent spin-phonon oscillations in the ferromagnetic van der Waals crystal CrI3. Presented at *MRS Spring/Fall meeting*, Boston, Massachusetts, United States, 2020-11-27 - 2020-11-27. (LA-UR-20-29296)

Saxena, A. B. Effect of Curvature on Topological Defects in Chiral Magnets and Soft Matter. Presented at *Curvilinear Magnetism*, Kiev, Ukraine, 2019-05-22 - 2019-05-22. (LA-UR-19-24633)

Saxena, A. B. Skyrmions and Hopfions: Chiral Magnets and Liquid Crystals. Presented at *MRS Spring Meeting*, Seattle, Washington, United States, 2021-04-19 - 2021-04-19. (LA-UR-21-23398)

Saxena, A. B. and A. Duzgun. Curvature Effects in Liquid Crystal Skyrmions. Presented at *WE-Heraeus-Seminar on"Curvilinear Condensed Matter"*, Hanau, Germany, 2021-06-24 - 2021-06-24. (LA-UR-21-25870)

Saxena, A. B. and S. Banerjee. Band Engineering in Lieb Lattice Geometry. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-22095)

Saxena, A. B. and S. Banerjee. Higher Chern Numbers and Quadratic Band Crossing Lines in Bilayer Lieb Lattice. Presented at *APS March Meeting*, Nashville, Tennessee, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22376)

Yuan, L. Tracking Charge and Energy Flow at the Nanoscale by Ultrafast Microscopy. . (LA-UR-21-31385)

Yuan, L., P. Jeong, K. Kwock, J. Schuck, D. A. Yarotski, I. Brener and R. P. Prasankumar. Manipulation of Exciton Dynamics and Annihilation by Enhanced Light-Matter Interaction in Single-Layer WSe2 on a Toroidal Dielectric Metasurface. Presented at *2020 CINT Annual Meeting (Virtual Conference)*, Albuquerque, Indiana, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27326)

Zhu, J. Electronic Correlation and Topology in f-Electron Quantum Matter. . (LA-UR-21-25821)

Zhu, J. Nonequilibrium quasiparticle dynamics in an unconventional superconductor with competing order. Presented at *PIPT7*, Santa Fe, New Mexico, United States, 2021-11-08 - 2021-11-17. (LA-UR-21-31381)

Zhu, J. Dark Matter Detection with Strongly Correlated Topological Matter: Flatband Effect. Presented at *Quantum Matter & Beyond*, Jacksonville Beach, Florida, United States, 2021-12-15 - 2021-12-17. (LA-UR-21-32248)

Fauseweh, B., S. Paeckel, A. Osterkorn, T. Koehler, D. Manske and S. Manmana. How can we detect superconductivity out of equilibrium?. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21944)

Fauseweh, B. and J. Zhu. Modeling the interplay of strong correlations and non-equilibrium excitation. Presented at *CINT Anual Meeting*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-24. (LA-UR-19-29382)

Fauseweh, B. and J. Zhu. Laser Pulse Driven Control of Charge and Spin Order in the two-dimensional Kondo Lattice. Presented at *CINT Annual Meeting*, Los Alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27028)

Padmanabhan, P., K. W. C. Kwock, A. Nedi\xc4\x87, T. V. Trevisan, S. Gilinsky, N. S. Sirica, J. Kim, K. Du, P. P. Orth, S. W. Cheong and R. P. Prasankumar. Giant Second Harmonic Generation from a Polar van der Waals Bismuth Telluro-Halide Semiconductor. Presented at *Photoinduced Phase Transitions 7*, Los Alamos, New Mexico, United States, 2021-11-10 - 2021-11-10. (LA-UR-21-31216)

Padmanabhan, P., S. Boubanga-Tombet, T. Otsuji and R. P. Prasankumar. Magnetoplasmonic manipulation of THz transmission and Faraday rotation using graphene micro-ribbon arrays. Presented at *Optical Terahertz Science and Technology*, Santa Fe, New Mexico, United States, 2019-03-10 - 2019-03-15. (LA-UR-19-22208)

Zhu, J. and B. Fauseweh. Nonequilibrium dynamics in the two-dimensional Kondo lattice model. Presented at *PIPT7*, Santa Fe, New Mexico, United States, 2021-11-08 - 2021-11-18. (LA-UR-21-31090)

enriquez, E., Q. Li, P. R. Bowlan, P. Lu, B. Zhang, L. Li, H. WANG, B. P. Uberuaga, D. A. Yarotski, R. P. Prasankumar, S. V. Kalinin, Q. JIA and A. Chen. Controlled Functionalities in Vertical Nanocomposites via Strain and Defect Engineering. . (LA-UR-19-24312)

enriquez, e., H. Han, P. C. Dowden and A. Chen. Advanced Thin Film Synthesis and Functionality Design Capabilities at CINT. . (LA-UR-19-24301)

Posters

Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials

Blas Uberuaga
20190043DR

Project Description

Testing of refurbished (aka Lifetime Extension), reused, or newly designed weapon components is central to the mission of the Enhanced Capabilities for Subcritical Experiments (ECSE) project. While the ECSE accelerator will produce an excellent x-ray sources that will be used for weapons radiography, a great deal of leverage (both in terms of cost and radiographic quality) comes from what happens in the radiographic imaging system. This project proposes to produce a new scintillator material, the most important component in the imaging system, that provides options to improve the performance of ECSE. Perhaps it goes without stating, but greater radiographic system performance for ECSE will vastly increase the value of the experiments performed there. Looking further afield, a deeper understanding of the important interplay between the atomic and condensed matter physics that determines scintillator performance will help us to improve these materials for other missions relevant to the National Nuclear Security Administration as well as Department of Energy writ large.

Technical Outcomes

This project has (a) demonstrated a closed loop between machine learning and experiment for the optimization of scintillators, (b) developed a hierarchy of physics-informed models to screen for new scintillator chemistries from millions of compounds, and (c) showed that band-edge engineering can mitigate the effects of radiation damage on performance. The team has identified one new compound that is being developed by other programs and a number of other candidates that require further investigation.

Publications

Journal Articles

B\xc3\xa1rta, J., K. S. Pestovich, J. A. Valdez, B. W. Wiggins, C. Richards, E. Smith, J. H. Clayton, D. Smalley and K. J. McClellan. Compositional screening of Ce-doped (Gd,Lu,Y)3(Al,Ga)5O12 ceramics prepared by quenching from melt and their luminescence properties. 2021. *Journal of Alloys and Compounds*. **889**: 161687. (LA-UR-21-20790 DOI: 10.1016/j.jallcom.2021.161687)

*Liu, X., G. Pilania, A. A. Talapatra, C. R. Stanek and B. P. Uberuaga. Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. 2020. *ACS Applied Materials & Interfaces*. **12** (41): 46296-46305. (LA-UR-20-24907 DOI: 10.1021/acsami.0c13236)

Morgan, D., G. Pilania, A. Couet, B. P. Uberuaga, C. Sun and J. Li. Machine learning in nuclear materials research. Submitted to *Current Opinion in Solid State & Materials Science*. (LA-UR-21-32380)

Pilania, G. Machine Learning in Materials Science: From Explainable Predictions to Autonomous Design. Submitted to *Computational Materials Science*. (LA-UR-20-28959)

*Pilania, G., A. Ghosh, S. T. Hartman, R. Mishra, C. R. Stanek and B. P. Uberuaga. Anion order in oxysulfide perovskites: origins and implications. 2020. *npj Computational Materials*. **6** (1): 71. (LA-UR-19-31746 DOI: 10.1038/s41524-020-0338-1)

Revi, V., S. Kasodariya, A. A. Talapatra, G. Pilania and A. Alankar. Machine Learning Elastic Constants of Multi-Component Alloys. Submitted to *Computational Materials Science*. (LA-UR-21-25687)

Sharma, V., P. Kumar, P. Dev and G. Pilania. Machine Learning Substitutional Defect Formation Energies in ABO3 Perovskites. Submitted to *Journal of Applied Physics*. (LA-UR-20-24008)

Singh, C. N., G. Pilania, J. Barta, B. P. Uberuaga and X. Liu. Accurately predicting optical properties of rare-earth scintillators: influence of electron-hole correlations. Submitted to *Journal of Materials Chemistry C*. (LA-UR-21-21690)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. A Machine Learning Approach to Prediction of Formability and Thermodynamic Stability of Single and Double Perovskite Oxides. Submitted to *Chemistry of Materials*. (LA-UR-20-25347)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Band gap predictions of Novel Double Perovskite Oxides

using Machine Learning. Submitted to *Chemistry of Materials*. (LA-UR-21-28459)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Supporting Information: Band gap predictions of Novel Double Perovskite Oxides using Machine Learning. Submitted to *Chemistry of Materials*. (LA-UR-21-28478)

Talapatra, A. A., D. Ghosh, B. P. Uberuaga and G. Pilania. Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. 2021. *Journal of Materials Science*. **56** (28): 15812-15823. (LA-UR-21-23719 DOI: 10.1007/s10853-021-06294-2)

*Thind, A. S., S. Kavadiya, M. Kouhnavard, R. Wheelus, S. B. Cho, L. Lin, C. Kacica, H. K. Mulmudi, K. A. Unocic, A. Y. Borisevich, G. Pilania, P. Biswas and R. Mishra. KBaTeBiO6: A Lead-Free, Inorganic Double-Perovskite Semiconductor for Photovoltaic Applications. 2019. *Chemistry of Materials*. **31** (13): 4769-4778. (LA-UR-19-25934 DOI: 10.1021/acs.chemmater.9b01025)

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

Wang, Z., K. Anagnost, C. W. Barnes, D. M. Dattelbaum, E. R. Fossum, E. Lee, J. Liu, J. J. Ma, W. Z. Meijer, W. Nie, C. M. Sweeney, A. C. Therrien, H. Tsai and X. Yue. Billion-pixel X-ray camera (BiPC-X) for wide field-of-view measurements. Submitted to *Review of Scientific Instruments*. (LA-UR-21-20086)

Conference Papers

Smith, E., B. W. Wiggins and C. G. Richards. Developments in garnet based scintillating composites for radiation detection applications. Presented at *SPIE Optics + Photonics*. (San Diego, California, United States, 2020-08-23 - 2020-08-27). (LA-UR-20-25861)

Books/Chapters

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

Reports

Wang, Z. Orbital ring and Dyson sphere from recycled space debris. Unpublished report. (LA-UR-21-21291)

Wang, Z. and Y. Shih. Entangled-photon interferometry for plasmas. Unpublished report. (LA-UR-21-23204)

Presentation Slides

Barta, J. High-throughput Synthesis and Characterization of Perovskites. Presented at *LDRD review for "Brigther, Faster, Tougher"*, Los Alamos, New Mexico, United States, 2020-02-19 - 2020-02-19. (LA-UR-20-21430)

Gehring, A. E., B. P. Uberuaga, T. J. Haines, J. Barta and B. W. Wiggins. Inorganic scintillator synthesis for targeted applications. . (LA-UR-20-20481)

Pestovich, K. S., C. J. Chandler, J. H. Clayton, B. P. Uberuaga and K. J. Mcclellan. Scintillator Discovery & Development within (Y,Lu,Gd)3(Al,Ga)5O12:Ce. Presented at *Scintillation Materials Research Center Research Group Meeting*, Knoxville, Tennessee, United States, 2020-09-14 - 2020-09-14. (LA-UR-20-27011)

Pilania, G. Materials that Glow: Discovering and designing new scintillators with machine learning. Presented at *Artificial Intelligence for Materials Science (AIMS) at NIST*, Gaithersburg, Maryland, United States, 2019-08-01 - 2019-08-01. (LA-UR-19-28296)

Pilania, G. Machine Learning for Materials Design An Example of Scintillator Discovery. Presented at *Artificial Intelligence for Material Design [online workshop]*, Mumbai, India, 2020-05-24 - 2020-06-09. (LA-UR-20-24311)

Pilania, G. A Machine-Learning-Based Strategy for Accelerated Discovery of Novel Scintillator Chemistries. Presented at *2020 VIRTUAL MRS SPRING FALL MEETING & EXHIBIT*, Los Alamos, New Mexico, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-29940)

Pilania, G. Annual Report Highlight Slides for w20_MatDesign. . (LA-UR-21-23502)

Pilania, G., A. Ghosh, S. T. Hartman, C. R. Stanek, R. Mishra and B. P. Uberuaga. Deciphering Anion Order in Oxysulfide Perovskites. Presented at *American Physical Society March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22004)

Rutstrom, D. J., M. Zhuravleva and K. J. Mcclellan. Evaluating New Double Perovskite Halide Scintillators for Radiation Detection Applications. . (LA-UR-21-28068)

Rutstrom, D. J. and K. J. Mcclellan. Summary of Summer Project: Evaluating New Double Perovskite Halide Scintillators for Radiation Detection Applications. . (LA-UR-21-28565)

Smith, E., C. G. Richards and B. W. Wiggins. Developments in garnet based scintillating composites for radiation detection applications. Presented at *SPIE Optics + Photonics*, San Diego, California, United States, 2020-08-24 - 2020-08-24. (LA-UR-20-26326)

Tafoya, L. R., V. Geppert-Kleinrath, K. J. Mcclellan, K. S. Pestovich and B. W. Wiggins. Investigation of proton-induced damage in Cerium doped mixed garnet scintillators. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27463)

Talapatra, A. A. A Machine-Learning based Hierarchical Screening Strategy to Expedite Search of Novel Scintillator Chemistries. Presented at *MRS Fall Meeting, 2019*, Boston, Massachusetts, United States, 2019-12-01 - 2019-12-06. (LA-UR-19-31946)

Talapatra, A. A. A Machine Learning Guided Discovery of Novel Oxide Perovskites for Scintillator Applications. Presented at *TMS 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-22212)

Talapatra, A. A. Accelerating scintillator materials discovery using Machine Learning. . (LA-UR-21-24920)

Talapatra, A. A. A Machine Learning aided hierarchical screening strategy for materials discovery. . (LA-UR-21-27531)

Talapatra, A. A. A Machine-learning Based Hierarchical Framework to Discover Novel Scintillator Chemistries. Presented at *Materials Science & Technology (MS&T 2021)*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-20. (LA-UR-21-30152)

Uberuaga, B. P. Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials. Presented at *MSTS Nevada Working Group*, Las Vegas, Nevada, United States, 2019-07-15 - 2019-07-17. (LA-UR-19-26531)

Uberuaga, B. P. Physics-Based Machine Learning Models for High Throughput Screening of Novel Scintillator Chemistries: Materials that Glow. Presented at *Materials Science & Technology 2019*, Portland, Oregon, United States, 2019-09-29 - 2019-09-29. (LA-UR-19-29653)

Uberuaga, B. P. Fundamental studies of radiation effects in materials. . (LA-UR-19-27963)

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

Uberuaga, B. P. Highlights performed on LANL IC on the project w19_matprops. . (LA-UR-21-24026)

Uberuaga, B. P., G. Pilania, K. J. Mcclellan and T. J. Haines. Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials. . (LA-UR-21-24063)

Wang, Z. Digital Twins for Scientific Cameras: Opportunities to enhance X-ray/neutron vision. Presented at *AIRES 2: Machine Learning for Robust Digital Twins (virtual*, Oak ridge, Tennessee, United States, 2021-01-19 - 2021-01-19. (LA-UR-21-20509)

Wang, Z. CMOS Radiography. Presented at *Disruptive Technology Workshop (Virtual*, Los Alamos, New Mexico, United States, 2021-02-24 - 2021-02-24. (LA-UR-21-21368)

Wang, Z., D. M. Dattelbaum, E. R. Fossum, G. Pilania, B. P. Uberuaga and UDA Collaboration. Towards Physics - informed cameras (PhI-Cam) for Flash X-ray Radiography. Presented at *22nd International Workshop on Radiation Imaging Detectors (IWoRID)*, Ghent, Belgium, 2021-06-27 - 2021-06-27. (LA-UR-21-25996)

Wang, Z., Z. He, P. Chu, M. R. James, J. L. Kiplinger, C. Morris, W. Nie, S. C. Vogel and E. B. Watkins. Neutron Radiography by a SIFaN Instrument. Presented at *OSA Imaging and Applied Optics Congress*, Vancouver, Canada, 2021-07-19 - 2021-07-19. (LA-UR-21-27439)

Posters

Pestovich, K. S., C. J. Chandler and K. J. Mcclellan. Development of Polycrystalline Scintillators to Screen New Compositions Predicted by Machine Learning. Presented at *2019 LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27704)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Machine-learning based discovery of novel oxide perovskites. Presented at *CONFERENCE ON A FAIR DATA INFRASTRUCTURE FOR MATERIALS GENOMICS [virtual conference]*, Los Alamos, New Mexico, United States, 2020-06-03 - 2020-06-05. (LA-UR-20-23932)

Talapatra, A. A. and R. Arroyave. Experiment Design Frameworks for Materials Discovery. Presented at *Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23119)

Williams, L., E. Kioupakis and G. Pilania. Machine Learning with Local Environment Descriptors to Predict New Scintillator Materials. Presented at *Michigan Institute for Computational Discovery in Engineering*, Ann Arbor, Michigan, United States, 2019-04-10 - 2019-04-10. (LA-UR-19-23018)

Other

Talapatra, A. A. A Machine Learning aided hierarchical screening strategy for materials discovery. Audio/Visual. (LA-UR-21-27864)

Accelerated Aging of Crystalline Plutonium Compounds

Justin Cross
20190228ER

Project Description

The goal of this project is to provide experimental data on the aging of well-defined, crystalline plutonium (Pu) salts by spiking 238Pu to produce significant radiation self-damage in a short, yet manageable, period of time. These data can then be used to answer the questions: i. What are the mechanisms of atom displacement and final product formation? ii. How resilient are the selected compounds and how long are they still useful? These results can be integrated into current and future efforts in material disposition, storage, and surveillance. Successful investigations can position the Labortaory as a leader in radiation damage of Pu compounds. This project will fill a gap of knowledge in the nuclear material management of the entire DOE complex as there are no studies on the degradation of crystalline salts with Pu as a main constituent. The findings will have high potential to inform a wide variety of unusual legacy residues that must be handled for future repackaging, storage, and/or disposition. This is especially pertinent with the recent resumption of shipments to the WIPP (Waste Isolation Pilot Plant). State-of-the-art radiological facilities, cutting edge spectroscopy, and access 238Pu place Los Alamos in the unique position to undertake this task.

Publications

Presentation Slides

Dan, D. Using Metal Organic Frameworks (MOFs) to Quantify the Abundance of Short-Lived Fission Products. . (LA-UR-21-30464)

Direct Plutonium-239 Nuclear Magnetic Resonance: A Unique Tool for Understanding Plutonium

Eric Bauer
20200045ER

Project Description

Understanding the chemical bonding of actinide materials is crucial for addressing important issues and finding solutions for problems across the Department of Energy (DOE) Nuclear Complex. Such issues include: controlling chemical processes for nuclear waste remediation and long-term storage, regulating reactivity for efficient actinide separation in reprocessing spent nuclear fuel, and for mitigation of actinide migration in the environment. To advance our understanding of the nature of bonding in the actinides, new spectroscopies must be developed and applied in order to control chemical bonding. We propose to develop of a capability for observing the plutonium-239 (Pu-239) Nuclear Magnetic Resonance signal in a variety of plutonium compounds to understand fundamental issues in actinide chemistry, in particular, bonding and electronic structure to help solve pressing problems facing the Nation.

Plutonium-239 Nuclear Magnetic Resonance Studies of Aging and Defects

Filip Ronning
20200125ER

Project Description

If successful, this project will result in a local probe of the physical and electronic structure of plutonium-based materials which are continuously evolving as a function of time due to the radioactive decay of plutonium. This could help shed light on the lifetime of the nuclear stockpile as well as with issues of waste storage.

Publications

Journal Articles

*Chiu, W., R. M. Tutchton, G. Resta, T. Lee, E. D. Bauer, F. Ronning, R. T. Scalettar and J. Zhu. Hybridization effect on the X-ray absorption spectra for actinide materials: Application to PuB4. 2020. *Physical Review B*. **102** (8): 085150. (LA-UR-20-21956 DOI: 10.1103/PhysRevB.102.085150)

Sakai, H., Y. Tokunaga, S. Kambe, F. Ronning, J. Zhu, J. D. Thompson, S. Ramakrishna, A. P. Reyes, K. Suzuki, Y. Oshima and M. Yokoyama. Nano-scale heterogeneity induced by non-magnetic Zn dopants in a quantum critical metal CeCoIn5: 115In NQR/NMR and 59Co NMR Study. Submitted to *Physical Review B*. (LA-UR-21-23885)

Presentation Slides

Zhu, J. Hybridization effect on the X-ray absorption spectra for actinide materials. Presented at *Virtual 2020 MRS Spring/Fall Meeting*, Boston, Massachusetts, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-28985)

Zhu, J., W. Chiu, R. M. Tutchton, G. Resta, T. Lee, E. D. Bauer, F. Ronning and R. Scalettar. Hybridization effect on the X-ray absorption spectra for actinide materials: Application to PuB4. Presented at *AVS 67*, Charlotte, North Carolina, United States, 2021-10-25 - 2021-10-28. (LA-UR-21-30174)

Dynamics of Quantum Phase Transitions

Wojciech Zurek
20200156ER

Project Description

The project aims at studying the formation of topological defects in symmetry-breaking phase transitions. It is a universal phenomenon relevant for many fields of physics, from cosmology to condensed matter. To achieve this goal we will (theoretically and experimentally) study the dynamics of quantum phase transitions in Bose-Einstein Condensate. The dynamics of quantum phase transitions is a topic that is important to areas of the Laboratory mission ranging from materials to quantum computing. In particular, quantum annealing used by D-Wave is a quantum phase transition. Indeed, the formation of defects during the evolution is a signature of errors in D-Wave. Our research will have an impact on Department of Energy (DOE) missions related to Quantum Information Science (QIS), where consideration is given to both how QIS can benefit DOE's and the Laboratory's Programs, and how Programs can benefit QIS.

Publications

Journal Articles

*Sadhukhan, D., A. Sinha, A. Francuz, J. Stefaniak, M. M. Rams, J. Dziarmaga and W. H. Zurek. Sonic horizons and causality in phase transition dynamics. 2020. *Physical Review B*. **101** (14): 144429. (LA-UR-19-30546 DOI: 10.1103/PhysRevB.101.144429)

Schmitt, M., M. M. Rams, J. P. Dziarmaga, M. Heyl and W. H. Zurek. Quantum phase transition dynamics in the two-dimensional Ising model. Submitted to *Nature Communications*. (LA-UR-21-24924)

Suzuki, F., M. Leneshko, W. H. Zurek and R. V. Krems. Localization of composite quantum particles in a random potential. Submitted to *Physical Review B*. (LA-UR-20-28806)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. 2022. *Physical Review Letters*. **128** (1): 010401. (LA-UR-21-20437 DOI: 10.1103/PhysRevLett.128.010401)

*Yan, B., V. Y. Chernyak, W. H. Zurek and N. A. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. 2021. *Physical Review Letters*. **126** (7): 070602. (LA-UR-20-26742 DOI: 10.1103/PhysRevLett.126.070602)

Yan, B., W. Chemissany and W. H. Zurek. Quantum Chaos on Complexity Geometry. Submitted to *Physical Review Letters*. (LA-UR-20-22063)

Zurek, W. H. Quantum Theory of the Classical: Einselection, Envariance, and Quantum Darwinism. Submitted to *Entropy*. (LA-UR-21-31822)

Zurek, W. H., A. Touil, B. Yan, D. Girolami and S. Deffner. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Submitted to *Physical Review Letters*. (LA-UR-21-25646)

Zurek, W. H., H. Zeng, C. ZIa and H. Zhang. Dynamics of spontaneous symmetry breaking in a holographic superconductor. Submitted to *Nature Physics*. (LA-UR-19-31918)

Zurek, W. H., M. M. Rams and J. Dziarmaga. Coherent Many-Body Oscillations Induced by a Superposition of Broken Symmetry States in the Wake of a Quantum Phase Transition. Submitted to *Physical Review Letters*. (LA-UR-22-20698)

Books/Chapters

Zurek, W. H. Conscious of a Classical World in a Quantum Universe. (LA-UR-20-28307)

Presentation Slides

Girolami, D., A. Touil, B. Yan, S. Deffner and W. H. Zurek. Quantitative limits to quantum correlations in many-body systems: a signature of classical objectivity. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21970)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21968)

Zurek, W. H. Dynamics of Quantum Phase Transitions. . (LA-UR-20-29719)

Zurek, W. H. Information Scrambling, Loschmidt Echo,and Decoherence. . (LA-UR-21-29934)

Plutonium Elasticity at Extreme Pressures using Gigahertz Ultrasound in a Diamond Anvil Cell

Blake Sturtevant
20200198ER

Project Description

Elemental plutonium exhibits one of the most complex phase diagrams in the periodic table. Understanding this phase diagram over a wide range of temperatures and pressures is of critical importance to the Laboratory's mission. Sound velocity and elasticity, which are fundamental thermodynamic properties, play an important role in constraining the equation of state of any material. Capabilities for the direct measurement of sound velocity are currently limited to pressures on the order of 10 gigapascal (GPa). This project will create an institutional capability to directly measure compressional and shear sound velocity simultaneously in a diamond anvil cell, where small samples (0.01 millimeter dimensions) are used to readily achieve pressures in excess of 100 GPa. This unique capability will be achieved by developing a novel dual mode ultra-high frequency acoustic transducer, where "dual-mode," refers to the ability to simultaneously generate shear and compressional acoustic waves. The dual-mode transducers will be designed using finite element methods and fabricated using standard microfabrication techniques. Simultaneous compressional and shear ultrasound measurements on actinide materials at high pressure will constitute successful completion of the project and provide vital information in support of Laboratory and National Nuclear Security Administration (NNSA) missions.

Publications

Presentation Slides

Couper, S. C. Material properties at ultrahigh pressures: developing a gigahertz ultrasound transducer for the diamond anvil cell. Presented at *Agnew and Metropolis Postdoc Fellow Showcase*, Los Alamos, New Mexico, United States, 2022-01-27 - 2022-01-27. (LA-UR-22-20599)

Posters

Couper, S. C. Material properties at ultrahigh pressures: developing a gigahertz ultrasound transducer for the diamond anvil cell. Presented at *Agnew and Metropolis Postdoc Fellow Showcase*, Los Alamos, New Mexico, United States, 2022-01-27 - 2022-01-27. (LA-UR-22-20598)

Predicting the Impact Sensitivity of New Explosives through Statistical Modeling

Virginia Manner
20200234ER

Project Description

The development of structure-process-performance relationships for the preparation of new energetic materials are crucial to future stewardship of the United States nuclear weapons stockpile, particularly as all future formulations will deviate in some way from those used in historical systems. Therefore, the ability to understand and manipulate the handling safety of new explosives would have a revolutionary effect on applications related to stockpile management, in addition to law enforcement and basic explosives research. Most explosives development is based on a costly trial-and-error approach with rounds of synthesis and testing because we cannot yet predict the properties of new high explosives. Theory and modeling rarely provide clear guidance for the explosive design process, in part because of the multitude of factors that influence handling safety. To address these deficiencies, we will mine historical Laboratory experimental data on high explosive sensitivity testing in order to make an exhaustive search of the properties of explosives that influence sensitivity, and use experimental tests and computational methods to fill in existing gaps in data. Finally, we will use statistical methods to analyze the large quantity of data and derive and validate rules for how to design and screen high explosives for handling safety.

Publications

Journal Articles

Burch, A. C., L. M. Klamborowski, J. D. Yeager, G. W. Brown, B. C. Tappan, M. J. Cawkwell and V. W. Manner. The effect of hardness on polymer-bonded pentaerythritol tetranitrate (PETN) explosive impact sensitivity. 2022. *Journal of Applied Physics*. **131** (1): 15102. (LA-UR-21-29423 DOI: 10.1063/5.0073867)

Cawkwell, M. J., A. C. Burch, J. V. Davis, S. R. Ferreira, N. M. Lease, F. W. I. Marrs and V. W. Manner. Understanding explosive sensitivity with effective trigger linkage kinetics. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-21-32237)

Cawkwell, M. J., A. C. Burch, S. R. Ferreira, N. M. Lease and V. W. Manner. Atom equivalent energies for the rapid estimation of the heat of formation of explosive molecules with density functional tight binding theory. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-20-21254)

Cawkwell, M. J., J. V. Davis, N. M. Lease, F. W. I. Marrs, A. C. Burch, S. R. Ferreira and V. W. Manner. Supplementary Material Understanding explosive sensitivity with effective trigger linkage kinetics. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-21-32470)

*I. Marrs, F. W., V. W. Manner, A. C. Burch, J. D. Yeager, G. W. Brown, L. M. Kay, R. T. Buckley, C. M. Anderson-Cook and M. J. Cawkwell. Sources of Variation in Drop-Weight Impact Sensitivity Testing of the Explosive Pentaerythritol Tetranitrate. 2021. *Industrial & Engineering Chemistry Research*. **60** (13): 5024-5033. (LA-UR-20-30351 DOI: 10.1021/acs.iecr.0c06294)

Books/Chapters

Cawkwell, M. J., S. R. Ferreira, N. M. Lease and V. W. Manner. Ranking explosive sensitivity with chemical kinetics derived from molecular dynamics simulations. (LA-UR-20-26693)

Presentation Slides

Burch, A. C., F. W. I. Marrs, J. V. Davis, J. D. Yeager, M. J. Cawkwell and V. W. Manner. Statistical analysis of large data sets to improve understanding of explosive sensitivity. Presented at *JANNAF*, online, New Mexico, United States, 2021-12-06 - 2021-12-16. (LA-UR-21-31580)

Manner, V. W. Hazard Analyses in Explosives Research and Career Paths. Presented at *Yale Chemistry Joint Safety Team and Professional Development Network*, New Haven, Connecticut, United States, 2021-05-14 - 2021-05-14. (LA-UR-21-24574)

I. Marrs, F. W. Influence networks in longitudinal bipartite relational data. Presented at *Joint Statistical Meetings*, Virtual, New Mexico, United States, 2021-08-08 - 2021-08-12. (LA-UR-21-26739)

Shedding Light on Quantum Phenomena in Topological Chiral Crystals

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Project Description

Within the past decade, topological materials have gone from an exotic curiosity to the subject of the 2016 Nobel Prize in Physics. Topological semimetals (TSMs) in particular exhibit a host of striking phenomena, giving them great promise for applications including quantum computing, quantum information, and spintronics. However, despite the intense effort in this burgeoning area, it has been hard to measure clear-cut signatures of material topology. This in turn has prevented these unique materials from realizing their vast potential for novel applications. Topological chiral crystals (TCCs) are a new class of materials with substantially improved properties that make measurements of previously elusive topological phenomena possible. Optical experiments can provide clear signatures of these phenomena, putting us in an excellent position to apply our extensive expertise in optical measurements on TSMs to TCCs. Our chief innovation is thus to combine our expertise in optical studies of TSMs with the availability of newly developed topological chiral crystals to clearly reveal signatures of topology. Our studies will thus establish the unique character of these systems, providing long awaited insight and comparison to theoretical predictions that sets the stage for future studies and applications of these fascinating materials.

Publications

Journal Articles

Chen, L., C. Setty, H. Hu, M. G. Vergniory, S. E. Grefe, A. Prokofiev, S. Paschen, J. Cano and Q. Si. Topological Semimetal driven by Strong Correlations and Crystalline Symmetry. Submitted to *Nature Physics*. (LA-UR-21-28235)

Grefe, S. E., Q. Si, H. Lai and S. Paschen. Extreme response of Weyl-Kondo semimetal to Zeeman coupling. Submitted to *Physical Review Letters*. (LA-UR-20-30516)

Sirica, N. S., P. Orth, M. Scheurer, Y. Dai, M. C. Lee, P. Padmanabhan, L. M. T. Mix, L. X. Zhao, G. Chen, B. Xu, R. Yang, B. Shen, C. C. Lee, H. Lin, S. A. Trugman, J. Zhu, N. Ni, X. G. Qiu, A. J. Taylor, D. A. Yarotski and R. P. Prasankumar. Photocurrent-driven transient symmetry breaking in the Weyl semimetal TaAs. Submitted to *Nature Materials*. (LA-UR-20-23580)

Sirica, N. S. and R. P. Prasankumar. Shaking up topology with light. Submitted to *Nature Materials*. (LA-UR-21-20965)

Presentation Slides

Grefe, S. E. Strongly correlated topological semimetals. Presented at *Electronic topology across the correlation spectrum*, Aspen, Colorado, United States, 2021-07-12 - 2021-07-30. (LA-UR-21-27196)

Grefe, S. E. The Weyl Kondo Semimetal. Presented at *Topological Materials: from weak to strong correlations - online 'stay in touch' meeting*, Online/Virtual, New Mexico, United States, 2021-08-04 - 2021-08-06. (LA-UR-21-27751)

Grefe, S. E. Extreme topological tunability of Weyl-Kondo semimetal to Zeeman coupling. Presented at *Part II - RCQM Workshop on Topological Materials and Electron Correlations*, Houston, Texas, United States, 2021-11-15 - 2021-11-17. (LA-UR-21-31390)

Grefe, S. E. Weyl-Kondo semimetal: Extreme topological tunability and nonlinear optical exploration. Presented at *American Physical Society (APS) March Meeting*, Virtual/Online, New Mexico, United States, 2022-03-13 - 2022-03-18. (LA-UR-22-22432)

Grefe, S. E., H. Lai, S. Paschen and Q. Si. Extreme response of Weyl-Kondo semimetal to Zeeman coupling. Presented at *2021 American Physical Society March Meeting (Virtual/Online)*, Virtual/Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22720)

Grefe, S. E., R. P. Prasankumar, Q. Si and J. Zhu. High harmonic generation in Weyl-Kondo semimetals. Presented at *2021 American Physical Society March Meeting (Virtual/Online)*, Online/Virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22719)

Grefe, S. E., S. Paschen, Q. Si and J. Zhu. Weyl-Kondo semimetals: extreme topological tunability and nonlinear optical signatures. Presented at *Strongly correlated electron systems 2020/21*, Online/Virtual, New Mexico, United States, 2021-09-27 - 2021-10-01. (LA-UR-21-29633)

Posters

Grefe, S. E. and J. Zhu. High-harmonic generation in a Weyl-Kondo semimetal. Presented at *Photoinduced Phase Transitions and Cooperative Phenomena*, Online/Virtual, New Mexico, United States, 2021-11-08 - 2021-11-19. (LA-UR-21-31211)

Sirica, N. S., P. Orth, M. Scheurer, R. Tobey, Y. Dai, M. C. Lee, P. Padmanabhan, L. M. T. Mix, S. Tietelbaum, M. Trigo, L. Zhao, G. Chen, B. Xu, R. Yang, B. Shen, C. Hu, C. C. Lee, L. Hsin, T. Cochran, P. R. Bowlan, A. K. Azad, S. A. Trugman, J. Zhu, M. Z. Hazan, N. Ni, X. Qiu, A. J. Taylor, D. A. Yarotski and R. P. Prasankumar. MANIPULATING ELECTRONIC SYMMETRY IN THE WEYL SEMIMETAL TaAs USING ULTRAFAST PHOTOCURRENTS. Presented at *CATS EFRC PI Meeting*, Ames, Iowa, United States, 2021-09-27 - 2021-09-27. (LA-UR-21-29519)

Other

Sirica, N. S., R. Y. Zhu, D. A. Yarotski and M. C. Lee. Optical pump-probe data on Weyl semimetals. Dataset. (LA-UR-20-24079)

Transition Metal Nitrides for Efficient Nitrogen Electrocatalysis

Rangachary Mukundan
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Project Description

Nitrogen reduction reaction (NRR) to produce ammonia by the Haber-Bosch (HB) process is leaving a significant carbon footprint and accounts for ~2% of global natural gas consumption and ~3% of greenhouse gas emissions. The electrochemical production of ammonia would not only solve this problem but also provide an additional way to store the energy from intermittent renewable electricity in a feedstock/fuel. The major challenge here is finding an effective catalyst for NRR since conventional precious metal-based catalysts suffer from competing hydrogen evolution reaction and catalysts with adequate selectivity have not been discovered. In this regard, transition metal nitrides (TMNs) have many advantages over metal catalysts as ammonia formation reaction occurs between the nitrogen on the nitride and adsorbed hydrogen, removing the need for pre nitrogen adsorption on the catalyst surface. We aim to prepare a variety of transition metal nitrides and evaluate their catalytic activity towards NRR in both aqueous and non-aqueous electrolytes. We will also develop the theoretical understanding of the NRR mechanism in these TMNs and develop design principles for the synthesis of efficient NRR catalysts.

Publications

Journal Articles

*Roads less traveled: Nitrogen reduction reaction catalyst design strategies for improved selectivity. 2021. *Current Opinion in Electrochemistry*. **28**: 100723. (LA-UR-20-25145 DOI: 10.1016/j.coelec.2021.100723)

Banerjee, A., B. M. Ceballos, C. Kreller, R. Mukundan and G. Pilania. A First Principles Investigation of Nitrogen Reduction to Ammonia on Zirconium Nitride and Oxynitride Surfaces. Submitted to *Journal of Materials Science*. (LA-UR-21-29531)

Young, S. D., A. Banerjee, G. Pilania and B. R. Goldsmith. Perovskite Oxynitrides as Tunable Materials for Electrocatalytic Nitrogen Reduction to Ammonia. Submitted to *Trends in Chemistry*. (LA-UR-21-26260)

Posters

Ramaiyan, K., S. Komini Babu, C. Kreller, R. Mukundan, Y. S. Kim, S. Maurya, F. H. Garzon, S. Ozden, A. Benavidez and D. Kelly. Electrochemical Synthesis of Ammonia Using Origami-like Molybdenum Carbide Nanoflakes As Nitrogen Reduction Reaction Catalyst. Presented at *GRC - Electrochemistry*, Ventura, California, United States, 2020-01-04 - 2020-01-10. (LA-UR-19-32701)

Design Principles for Skyrmions in f-electron Materials

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Project Description

Skyrmions are particle-like objects stabilized in magnets. They are promising candidates for next-generation memory devices. It is desirable to expand the skyrmion-materials in order to optimize skyrmion properties. This research will reveal a novel mechanism for skyrmion stabilization in f-electron materials. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion materials and spintronics.

Publications

Journal Articles

Banerjee, S., U. Kumar and S. Lin. Inverse Faraday effect in Mott insulators. Submitted to *Physical Review Letters*. (LA-UR-21-28801)

Jeong, J., S. Lin, Y. Lee, C. Lee, J. W. Choi, Y. H. Jeong, H. J. Chang and J. Kim. Hard skyrmions in a rare earth permanent magnet. Submitted to *Nature Communications*. (LA-UR-19-31929)

Li, Z., J. Su, S. Lin, D. Liu, Y. Gao, S. Wang, H. Wei, T. Zhao, Y. Zhang, C. Jianwang and B. G. Shen. Field-free magnetic topology transformation in the domain wall of ferrimagnetic GdFeCo. Submitted to *Nature Nanotechnology*. (LA-UR-20-27806)

Lin, S. Skyrmion lattice in centrosymmetric magnets with local Dzyaloshinsky-Moriya interaction. Submitted to *Scipost Physics*. (LA-UR-21-32483)

Seo, S., S. Hayami, Y. Su, S. M. Thomas, F. Ronning, E. D. Bauer, J. D. Thompson, S. Lin and P. Ferrari Silveira Rosa. Spin-texture-driven electrical transport in multi-Q antiferromagnets. Submitted to *Nature Communications*. (LA-UR-20-24023)

Wang, Z., H. Zhou, M. Guo, L. Zhao, T. Xu, Y. Dong, K. Wu, S. G. Je, W. Chao, M. Im, H. Han, S. Lee, K. Lee, C. Song, H. Wu, S. Lin and W. Jiang. Thermal generation, manipulation and detection of skyrmions. Submitted to *Nature Electronics*. (LA-UR-19-25918)

*Wang, Z., Y. Su, S. Lin and C. D. Batista. Skyrmion Crystal from RKKY Interaction Mediated by 2D Electron Gas. 2020. *Physical Review Letters*. **124** (20): 207201. (LA-UR-19-31876 DOI: 10.1103/PhysRevLett.124.207201)

Zhao, X., J. Tang, K. Pei, W. Wang, S. Lin, H. Du, M. Tian and R. Che. Deterministic generation of skyrmions and antiskyrmions by electric current. Submitted to *Nature Nanotechnology*. (LA-UR-21-20900)

*Zhentao, W., S. Ying, L. Shi-Zeng and C. D. Batista. Meron, skyrmion, and vortex crystals in centrosymmetric tetragonal magnets. 2021. *Physical Review B*. **103** (10): 104408. (LA-UR-20-29175 DOI: 10.1103/PhysRevB.103.104408)

Presentation Slides

Lin, S. Topology and its electrical current control in two dimensional Moir\xc3\xa9 superlattice. Presented at *Wutong Forum of The Chinese University of Hong Kong*, Shenzhen, China, 2021-08-14 - 2021-08-15. (LA-UR-21-28150)

Lin, S., S. M. Thomas and P. Ferrari Silveira Rosa. LDRD appraisal: Design Principles for Skyrmions in f- electron Materials. . (LA-UR-20-29340)

Saxena, A. B. Hopfions in Anisotropic Heisenberg Magnets. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-14. (LA-UR-22-21627)

Posters

Lin, S. Topological spin texture in centrosymmetric magnets. Presented at *VI International Workshop Dzyaloshinskii-Moriya Interaction and Exotic Spin Structures*, Vyborg, Russia, 2021-09-06 - 2021-09-06. (LA-UR-21-28964)

Zhu, J., A. Ghosh and S. Lin. Data-driven study of magnetic interactions of transition-metal based 2D materials. Presented at *2020 APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-19-30770)

Pushing Past the 100 Tesla Threshold: Designing a High Conductivity/High Strength Metallic Composite Conductor

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Project Description

Energy security is of critical interest to the Department of Energy (DOE) and is one of the three main missions for Los Alamos National Laboratory. This project will develop a new metallic nanocomposite material that will enable an increase in the upper limit of magnetic fields of 100 Tesla (T) to 120 T. Currently magnetic fields are used to characterize or look at a wide variety of energy related materials such as high temperature superconductors. For the case of high temperature superconductive materials, the underlying mechanism of electron pairing remains unknown although decades have passed since the discovery of this phenomenon. Currently, we lack magnetic fields sufficient to suppress superconductivity for the materials in which the pairing is strongest. Magnetic fields beyond 100 T would enable study of the pairing interaction that is essential for development of future high temperature superconducting materials. Understanding this phase transition would enable development of near-room-temperature superconductive materials that would reinvent our current energy grid. This reinvention would be enabled by removing the resistance in the power lines that transition power from plants to homes. This increases efficiency of distribution for all power sources from wind to nuclear to coal.

Publications

Journal Articles

Blaschke, D., J. S. Carpenter, A. Hunter, C. Miller, E. L. Tegtmeier and W. P. I. Winter. Predicting electrical conductivity in Cu/Nb composites: a combined model-experiment study. Submitted to *TBD*. (LA-UR-21-30714)

Blaschke, D., J. S. Carpenter, A. Hunter, C. Miller, E. L. Tegtmeier and W. P. I. Winter. Predicting electrical conductivity in Cu/Nb composites: a combined model-experiment study. Submitted to *TBD*. (LA-UR-21-30714)

Blaschke, D., J. S. Carpenter, A. Hunter, C. Miller, E. L. Tegtmeier and W. P. I. Winter. Predicting electrical conductivity in

Cu/Nb composites: a combined model-experiment study. Submitted to *TBD*. (LA-UR-21-30714)

Carpenter, J. S., D. J. Savage, C. Miller, R. J. Mccabe, S. Zheng, D. R. Coughlin and S. C. Vogel. Accumulative Roll Bonding of Alloy 2205 Duplex Steel and the Accompanying Impacts on Microstructure, Texture, and Mechanical Properties. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-22-22594)

Carpenter, J. S., E. L. Tegtmeier, W. P. I. Winter, C. Miller and D. Coughlin. The Impact of Rolling at Temperature on Conductivity and Texture in Nanolamellar Cu/Nb Bimetallic Composites. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-21-31438)

Ma, X., B. Gwalani, J. Tao, M. Efe, M. Olszta, M. Song, S. Yadav, A. Yu, T. J. Nizolek, J. S. Carpenter, B. Zhou, A. Devaraj, S. Mathaudhu and A. Rohatgi. Shear strain gradient in Cu/Nb nanolaminates: strain accommodation and chemical mixing. Submitted to *Acta Materialia*. (LA-UR-21-31147)

H. A. *. B. I. J. *. L. R. A. *. D. K. *. M. E. Peng, X. *., A. Hunter, R. A. Lebensohn and X. Peng. Non-orthogonal computational grids for studying dislocation motion in phase field approaches. 2021. *Computational Materials Science*. **200**: 110834. (LA-UR-21-25715 DOI: 10.1016/j.commatsci.2021.110834)

Emergent Infrared Localized Surface Plasmon Resonances in Doped Spinel Metal Oxide Nanomaterials

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Project Description

Near-infrared light (IR) is the foundation of fiber-optics based telecommunication technologies (1300-1550 nanometer). The range of communications and information technologies impacted by IR light sources, and the resulting market for IR solid-state lighting (SSL) sources—light-emitting diodes (LEDs) and laser diodes—is expected to dramatically expand over the next 5 years. These include LEDs for proximity sensors, eye tracking and gesture recognition and lasers for optical communication, Light Detection and Ranging (LIDAR) in automotive applications and 3-Dimensional facial recognition. The ability to miniaturize light sources and to easily integrate with portable/wearable/fabric technologies is key. Nanosized plasmonic materials developed here, when coupled with nanosized quantum emitters, promise new solid-state miniaturized light sources for all of these applications, which will will be critical components in a range of light-enabled, global security-relevant technologies.

Publications

Journal Articles

Dolgopolova, E., D. Li, J. D. Watt, C. Ocampo, J. Hu, R. Kukkadapu, J. L. Casson, R. Bose, A. V. Malko, A. V. Blake, S. A. Ivanov, H. Htoon, H. Chen, G. Pilania and J. A. Hollingsworth. Spinel Fe3O4 Nanocrystals With Size-Tunable Plasmonic Properties Afford Strong Enhancement of Emission at Telecom Wavelengths. Submitted to *Journal of the American Chemical Society*. (LA-UR-20-28261)

Dolgopolova, E., D. Li, S. T. Hartman, J. D. Watt, C. Rios, H. Juejun, R. K. Kukkadapu, J. L. Casson, R. Bose, A. V. Malko, A. V. Blake, S. A. Ivanov, O. Roslyak, A. Piryatinski, H. Chen, G. Pilania and J. A. Hollingsworth. Strong Purcell Enhancement at Telecom Wavelengths Afforded by Spinel FeO Nanocrystals with Size-Tunable Plasmonic Properties. Submitted to *Nanoscale Horizons*. (LA-UR-21-30232)

Hartman, S. T. and G. Pilania. Defect Thermodynamics in Spinel Oxides Leading to Plasmonic Behavior. Submitted to *ACS Photonics*. (LA-UR-21-31746)

Presentation Slides

Dolgopolova, E. and J. A. Hollingsworth. Alternative plasmonic nanomaterials as building blocks for Purcell-enhanced emission in the infrared. Presented at *2020 Spring ACS National Meeting, COLL Virtual Technical Symposium*, Los Alamos, New Mexico, United States, 2020-03-22 - 2020-03-24. (LA-UR-20-22500)

Dolgopolova, E. and J. A. Hollingsworth. Alternative nanomaterials with size-dependent plasmonic properties for Purcell-enhanced emission in the infrared. Presented at *ACS Fall 2020 Virtual Meeting*, San Francisco, California, United States, 2020-08-16 - 2020-08-16. (LA-UR-20-26512)

Hartman, S. T., E. Dolgopolova, G. Pilania and J. A. Hollingsworth. Theory-Guided Identification and Development of Plasmonic Spinel Oxides. Presented at *American Physical Society March Meeting*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22454)

Hollingsworth, J. A. Advanced Quantum Emitters: Chemistry, Photophysics, Integration and Application. . (LA-UR-21-24265)

Hollingsworth, J. A. Quantum Dots: From Precision Synthesis to High-Tech Applications in National Security—Part 2. . (LA-UR-21-26228)

Hollingsworth, J. A. Nano-Enabled Single-Photon Sources for Quantum Applications. Presented at *nanoGe SpringMeeting*, Virtual (international), Spain, 2022-03-07 - 2022-03-11. (LA-UR-22-22234)

Hollingsworth, J. A. and E. L. E. McNesby. Synthesizing plasmonic shell PbS/CdS/CuxS quantum dots to enhance emission rates. . (LA-UR-21-27813)

Pilania, G. High throughput ab-initio and molecular dynamics studies of functional materials. . (LA-UR-22-22262)

Posters

Dolgopolova, E., D. Li, J. D. Watt, G. Pilania, C. Ocampo, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Alternative Plasmonic Nanomaterials for Purcell-Enhanced Emission in the Infrared Region. Presented at *CINT Annual*

Meeting, Online, New Mexico, United States, 2020-09-21 - 2020-09-24. (LA-UR-20-27165)

Measurement of Dynamic Friction via Kolsky Bar

Benjamin Morrow
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Project Description

Friction data, especially at high rates (dynamic friction), is sparse or completely unavailable for many Laboratory-relevant materials. As a result, computational models to describe friction tend to be underdeveloped and unvalidated, decreasing confidence in simulation results. This project seeks to remedy this by 1) developing the capability to measure dynamic friction without expensive and time-consuming modifications to existing test systems, 2) validate the test technique by performing measurements at quasi-static and dynamic rates; compare with known values when possible, and generate new data where legacy testing is unavailable, and 3) mature and validate the friction models developed for a Laboratory hydrocode that is used to simulate engineering systems, improve predictive capability if necessary, and use simulations to streamline analysis of experimental tests. This program will directly contribute to filling existing gaps in experimental data, and has the potential to greatly reduce both experimental and computational uncertainties for Laboratory missions such as Stockpile Stewardship, Science Campaigns, Joint Munitions Program, and others.

Publications

Journal Articles

*EUSER, V. K., D. L. WILLIAMSON, A. J. CLARKE and J. G. SPEER. Limiting Retained Austenite Decomposition in Quenched and Tempered Steels: Influences of Rapid Tempering and Silicon. 2020. *ISIJ International*. **60** (12): 2990-3000. (LA-UR-20-23093 DOI: 10.2355/isijinternational.ISIJINT-2020-263)

Euser, V. K., A. J. Clarke and J. G. Speer. Rapid Tempering: Opportunities and Challenges. Submitted to *Journal of Materials Engineering and Performance*. (LA-UR-20-24087)

Euser, V. K., D. L. Williamson, K. O. Findley, A. J. Clarke and J. G. Speer. The Role of Retained Austenite in Tempered Martensite Embrittlement of 4340 and 300-M Steels Investigated through Rapid Tempering. Submitted to *Metals*. (LA-UR-21-27333)

Conference Papers

Euser, V. K., A. B. Goodbody, C. A. Yablinsky, N. A. Denissen and B. M. Morrow. Design and Simulation of Insert to Measure Dynamic Sliding Friction in a Split-Hopkinson Pressure Bar. Presented at *Dymat*. (Madrid, Spain, 2021-09-20 - 2021-09-24). (LA-UR-21-23362)

Reports

Euser, V. K., N. A. Denissen, C. A. Yablinsky and B. M. Morrow. Literature Review on the Theory and Measurement of Dry Sliding Friction of Metals. Unpublished report. (LA-UR-20-29397)

Presentation Slides

Euser, V. K., A. J. Clarke, K. O. Findley and J. G. Speer. Rapid Tempering of Quenched Martensite. Presented at *Thermec 2021*, Los Alamos, New Mexico, United States, 2021-05-11 - 2021-05-11. (LA-UR-21-21730)

Euser, V. K., B. M. Morrow, C. A. Yablinsky and N. A. Denissen. Measurement of Dynamic Friction via Kolsky Bar. . (LA-UR-21-25499)

Euser, V. K., C. A. Yablinsky, N. A. Denissen and B. M. Morrow. Co-development of Experiment and Simulation to Observe Dynamic Behavior in Metals in Complex Loading Environments. Presented at *MS&T 21*, Columbus, Ohio, United States, 2021-10-18 - 2021-10-18. (LA-UR-21-30092)

Euser, V. K., C. P. Trujillo, C. Liu, A. B. Goodbody, C. A. Yablinsky, N. A. Denissen and B. M. Morrow. Design and Simulation of Insert to Measure Dynamic Sliding Friction in a Split-Hopkinson Pressure Bar. Presented at *Dymat 2021 - 13th INTERNATIONAL CONFERENCE on MECHANICAL and PHYSICAL BEHAVIOUR of MATERIALS under DYNAMIC LOADING*, Madrid, Spain, 2021-09-20 - 2021-09-24. (LA-UR-21-29003)

Morrow, B. M., V. K. Euser, C. A. Yablinsky and N. A. Denissen. Measurement and Simulation of Dynamic Friction via Kolsky Bar Technique. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-21559)

Defects and Functional Interfaces for Desalination

Jacob Spendelow
20200425ER

Project Description

Access to potable water in the face of a changing climate is a key challenge facing the Department of Energy (DOE). The goal of the project is to develop cost effective desalination technology. The work involves utilizing novel structures to remove the salt from sea water effectively by adsorbing the salt on the electrode surface. The enhancements from the novel structures is projected to provide up to a 100% increase in capacity over state of the art, which could transform the desalination industry. The improved desalination technology could also enable drinking water in marine and off-shore application which are of interest to the Department of Defense (DOD).

Publications

Journal Articles

Chen, L., Q. Kang and W. Q. Tao. Pore-scale study of coupled multiphase flow and reactive transport processes in catalyst layers of proton exchange membrane fuel cells. Submitted to *International Journal of Heat and Mass Transfer*. (LA-UR-20-22352)

Liu, M., Q. Kang, S. Komini Babu, J. B. Waugh and J. S. Spendelow. Numerical modeling of ion transport and adsorption in porous media: A pore-scale study for capacitive deionization desalination. 2022. *Desalination*. **526**: 115520. (LA-UR-20-25564 DOI: 10.1016/j.desal.2021.115520)

*Zhao, J., F. Qin, D. Derome, Q. Kang and J. Carmeliet. Improved pore network models to simulate single-phase flow in porous media by coupling with lattice Boltzmann method. 2020. *Advances in Water Resources*. **145**: 103738. (LA-UR-20-21321 DOI: 10.1016/j.advwatres.2020.103738)

Zhao, J., F. Qin, Q. Kang, C. Qin, D. Derome and J. Carmeliet. A dynamic pore network model for imbibition simulation considering corner film flow. Submitted to *Water Resources Research*. (LA-UR-21-32185)

Presentation Slides

Komini Babu, S., R. Mukundan, J. S. Spendelow and A. Yilmaz. PTL Development and Characterization at LANL. Presented at *H2NEW- AMP*, Los Alamos, New Mexico, United States, 2022-03-30 - 2022-03-30. (LA-UR-22-22576)

Kang, Q. Institutional computing project annual report: Figures. . (LA-UR-22-21708)

Waugh, J. B., J. S. Spendelow and S. Komini Babu. John Waugh Qualifying Exam Presentation. Presented at *John Waugh Qualifying Exam Presentation, virtual*, Santa Fe, New Mexico, United States, 2021-08-16 - 2021-08-16. (LA-UR-21-28164)

Waugh, J. B., S. Komini Babu and J. S. Spendelow. Hierarchical Porosity in Electrospun Capacitive Deionization Electrodes. Presented at *ECS Meeting*, Atlanta, Georgia, United States, 2021-10-10 - 2021-10-14. (LA-UR-21-30487)

Synchrotron-based High-Energy Proton Radiography

Matthew Freeman
20200644ER

Project Description

We presently utilize a suite of radiographic diagnostics to probe dense, dynamic systems in pursuit of a greater understanding of their behavior. Within these capabilities, certain gaps exist, either in the available resolution, depth of material penetration, or in the available timing between image acquisitions, that leaves many questions about the expected behavior of materials unanswered. This work will evaluate a new technique that bridges some of these gaps between capabilities, by deploying proton radiography at a synchrotron facility in Germany with characteristics uniquely suited to help probe some of these unknowns. The capabilities that this would add include a factor-of-five higher proton energy that will enable the probing of denser, thicker slabs of material, as well as a x100 increase in the available protons per pulse, which will enable high fidelity imaging of very subtle effects that are presently very difficult to characterize using radiographic probes. The establishment of a collaborative effort at this early stage in the development of this new facility will pave the way towards a future collaborative effort that will yield valuable scientific results for years to come.

Publications

Reports

Freeman, M. S. PRIOR: Proton Microscope for FAIR. Shock Wave Experiements with PRIOR.. Unpublished report. (LA-UR-20-25617)

Presentation Slides

Freeman, M. S. Developments in the Development of the OMEGA Electron Radiography HED Diagnostic – Part II. Presented at *42nd International Workshop on High Energy-Density Physics with Intense Laser Beams*, Online, New Mexico, United States, 2022-02-01 - 2022-02-01. (LA-UR-22-20848)

Electrically Pumped Laser Processed from Solution

Victor Klimov
20210176ER

Project Description

This project addresses a still unresolved challenge of practically realizing an electrically pumped laser with a solution processable gain medium. The availability of such lasers would benefit numerous existing and emerging technologies including integrated electronics and photonics, optical interconnects, lab-on-a-chip platforms, wearable devices, and neuromorphic computing. Presently, several National Funding Agencies (including Department of Homeland Security, National Science Foundation, and Department of Defense) are actively pursuing new programs in areas of on-chip optical gain media and on-chip lasers as a means to enable further complexity in highly integrated electronic circuits, enhance scalability in traditional and quantum photonic circuits and push sensitivity limits in on-chip diagnostics for detecting chemical and biological hazards.

Publications

Journal Articles

*Jung, H., N. Ahn and V. I. Klimov. Prospects and challenges of colloidal quantum dot laser diodes. 2021. *Nature Photonics*. **15** (9): 643-655. (LA-UR-21-22207 DOI: 10.1038/s41566-021-00827-6)

Understanding How Exploding Bridge-Wire (EBW) Detonators Work

Philip Rae
20210189ER

Project Description

There are several detonator technologies of interest to the National Nuclear Security Administration. The oldest, exploding bridgewire (EBW) detonators, are amongst the least understood in terms the fine details of how they actually work. This project aims to dig into the weeds of how they actually function, both to solve the 75 year old scientific mystery and also possibly allow new, better or safer detonators to be designed based on this new knowledge.

Publications

Journal Articles

Feagin, T. A., E. M. Heatwole, P. J. Rae, R. C. Rettinger and G. R. J. Parker. Time-Resolved Nanosecond Optical Pyrometry of the Vapor to Plasma Transitions in Exploding Bridgewires. Submitted to *Scientific Reports*. (LA-UR-21-20261)

Rae, P. J. The modeling of weak shock waves in highly porous powder beds and comments on its relevance to exploding bridgewire (EBW) detonators. Submitted to *Shock Waves*. (LA-UR-20-29268)

Rae, P. J. The action-integral and energy to explode short gold wires in ambient air. Submitted to *Physics of Plasmas*. (LA-UR-20-30296)

Rae, P. J. and R. C. Rettinger. The effects of electrically exploding gold bridgewires into inert and explosive powder beds. Submitted to *Shock Waves*. (LA-UR-21-23993)

High-Efficiency Steam Electrolysis Using Polymer Electrolyte Membranes

Yu Seung Kim
20210227ER

Project Description

Hydrogen enables resiliency, energy security, and economic growth across multiple sectors, including renewable and grid electricity. Hydrogen can be produced from diverse domestic feedstocks using a variety of process technologies, including natural gas, coal, nuclear power, and renewable resources. One of the most promising technologies to produce green hydrogen is water electrolysis. Several water electrolysis technologies at the temperature range of 30 to 80 degrees Celsius (C) are under development from early-stage research sponsored by the Department of Energy (DOE), Hydrogen and Fuel Cell Technologies Office. However, those low-temperature electrolysis technologies have low hydrogen production efficiency due to the low operating temperature. In this project, we aim to develop novel conducting materials that enable the operation of water electrolysis at the temperature range of 100 to 200 degrees C. The proposed steam electrolyzer may address the limitations of current water electrolysis technologies by having increased reaction kinetics, higher efficiency and faster hydrogen production rate.

Ultrafast control of material properties through shallow-core electrons

Pamela Bowlan
20210290ER

Project Description

As the energy demands of our nation increase, there is a strong need for fundamentally different technology for accessing material properties on demand, for faster more efficient computation and data storage. The idea proposed here, to use femtosecond extreme ultraviolet light pulses for controlling observable material properties such as magnetism and ferroelectricity, offers a novel approach with the potential to be orders of magnitude faster than electronic means of switching. Studying quantum materials with femtosecond extreme ultraviolet light pulses also offers a unique tool for understanding the role of the core electrons and the lattice in leading to a observable properties, which can give to new insight into how to access novel states of matter in the steady state or transiently. The free-electron laser and table top methods that will be developed in this project are also relevant to studying any materials in extreme conditions. Therefore this project has the potential to put Los Alamos National Laboratory at the forefront of quantum materials research and contribute new methods for studying materials in extreme conditions.

Publications

Presentation Slides

Peters, W., T. N. Jones, S. Song, M. Chollet, J. Robinson, L. Foglia, F. Bencivenga, R. Coffee and P. R. Bowlan. X-ray–optical transient grating measurements at LCLS. Presented at *Conference on Light and Electro-Optics (CLEO*, virtual, California, United States, 2021-05-09 - 2021-05-09. (LA-UR-21-24465)

Unconventional superconductivity in the Nickelates

Mun Chan
20210320ER

Project Description

High-temperature superconductivity is an emergent electronic state of matter that permits perfect conduction of electricity. It is an essential property for future power-grid applications, magnet-technology, and is the foundation for ideas concerning quantum computing. Despite decades of research, it remains one of the greatest unsolved problems in physics. The 2019 discovery of superconductivity in infinite layer nickelate opens a new family of unconventional superconductors for study. This project aims to achieve a fundamental understanding of this new material.

Publications

Presentation Slides

Maiorov, B. A. New discoveries and opportunities for superconductors in pulsed-high magnetic fields. Presented at *CEC-ICMC 21*, virtual conference, New Mexico, United States, 2021-07-19 - 2021-07-23. (LA-UR-21-26685)

Maiorov, B. A. New discoveries and opportunities for superconductors in high magnetic fields: What can we learn above 40T?. Presented at *Internal Seminar*, Los Alamos, New Mexico, United States, 2021-09-09 - 2021-09-09. (LA-UR-21-28897)

Maiorov, B. A. Challenges and opportunities for Superconductors in High Magnetic Fields. . (LA-UR-21-31299)

Hybrid Thermochromic Nanostructures for Radiative Heat Emergent Functionalities

Wilton Junior de Melo Kort-Kamp
20210327ER

Project Description

Reducing human reliance on energy-inefficient thermal management systems has taken on renewed urgency to reduce carbon emissions on our warming planet. Particularly, accomplishing environmentally friendly materials for temperature control would strongly impact the United States' energy landscape, where heating and cooling of residential and commercial structures account for about one-third of the electricity use, making them the largest energy expense in the country. The key innovation of this project is to develop phase-change nanostructured materials that passively monitor the ambient temperature and autonomously switch between absorber and emitter states to maintain the temperature close to a desired set point without any energy consumption. Our material platform could solve critical challenges in radiative heat phenomena, including passive radiative cooling technologies, artificial thermal skins for personal temperature regulation, and thermal sensing. Scaled up production of our proof-of-concept metasurfaces could help promote thermochromic photonic systems as a viable energy technology with clear applications to temperature regulation in residential and commercial structures in harsh climates, mitigation of material stresses on structures undergoing thermal cycles, and passive thermal management of micro-satellites. This project will have a positive impact to national energy security as well as strongly impact research in renewable energy, nanotechnology, and nanophotonic sciences.

Publications

Journal Articles

Sanders, S., L. Zundel, W. J. de Melo Kort-Kamp, D. A. R. Dalvit and A. Manjavacas. Near-Field Radiative Heat Transfer Eigenmodes. Submitted to *PRL*. (LA-UR-21-20930)

*Szilard, D., P. Abrantes, F. Pinheiro, F. Rosa, C. Farina and W. J. de Melo Kort-Kamp. Optical Forces on an Oscillating Dipole Near VO2 Phase Transition. 2021. *Universe*. **7** (6): 159. (LA-UR-21-23943 DOI: 10.3390/universe7060159)

Presentation Slides

Singh, L., E. B. Qiu, A. E. Cardin, A. Chen, D. A. R. Dalvit, I. K. Schuller, T. S. Luk, A. J. Schuller, W. J. de Melo Kort-Kamp and A. K. Azad. Nanophotonic metasurface for a novel thermal management system. Presented at *American Physical Society (APS) March Meeting*, chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22235)

Dynamic Catalysis, Advancing Beyond the Sabatier Principle

Ulises Martinez
20210345ER

Project Description

Our work targets the delivery of scientific discovery and technical breakthroughs in support of Department of Energy and National Nuclear Security Administration missions. Particularly, this project will create a solid foundation for the design of next-generation electrocatalysts with controlled functionality directly applicable to a wide range of Los Alamos National Laboratory programs in electrochemical energy conversion/storage including fuel cells, electrolyzers, batteries, as well as other applications such as chemical synthesis through carbon dioxide (CO_2)-electroreduction and electrochemical ammonia synthesis. This project focuses on controlled functionality and predictable performance through the discovery of fundamental material properties with theory-guided innovation at the boundaries of chemistry, physics, and materials science. Our team seeks to create the capability to enable process-to-performance design rooted in fundamental science through advancing our understanding of mechanisms, rates, and performance of materials.

Publications

Presentation Slides

Chavez Atayde, L. A. and U. Martinez. Dynamic (Electro)Catalysis: Advancing Beyond the Sabatier Principle. . (LA-UR-21-31952)

Martinez, U., C. M. Benway, L. A. Chavez Atayde, L. C. Delfin Manriquez, T. G. Segni, V. Chillara and E. F. Holby. Effects of Electromagnetic Waves on Electrochemical Systems. Presented at *LANL Summer Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27667)

Predicting and Controlling Interfacial Defects in Soft Matter

Matthew Lee
20210362ER

Project Description

We will develop both the theoretical understanding needed and the technological tools required to control morphological development during real-world polymer processing. We will apply both time-resolved structural characterization during 3-Dimensional printing and a new theoretical method for predicting mesoscale organization. As a result, we will have the ability to fabricate new materials with combinations of properties that are currently unavailable using traditional manufacturing techniques, and we will significantly improve the contribution of additive manufacturing to the new field of polymer upcycling (the process of converting discarded plastics into higher-value materials). In addition, the small footprint and relatively low costs associated with most polymer-based additive manufacturing methods allow for distributed manufacturing; combining this factor with our proposed capability would enable a quick local response to materials needs that arise urgently, e.g., as a result of supply chain interruptions or for production of supplies in remote locations. This project will provide a basis grounded in physics for quickly formulating new feedstocks with imperfect materials.

Manipulating Gas-Phase Chemistry in High Explosive Thermal Decomposition

Amanda Duque
20210399ER

Project Description

We recently discovered that our current understanding of thermal ignition of energetic materials may need to be revised -- we observed that the presence of strong electromagnetic (EM) fields significantly alters the fundamental thermal decomposition of a common stockpile high explosive (HE), 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX). This project takes an experimental and modeling approach to uncover the details of this interaction so that we may quantify and predict this behavior for a wide range of energetic materials. We are exploring new and original concepts – compared to traditional thermal effects, almost nothing is known about how EM energy interacts with explosives. For the first time, we will establish a physical-based connection between the materials and explosive properties from the microscale to the bulk continuum response, ultimately to predict and strategically utilize this phenomenon in a broader range of HE systems. The results from this project will not only provide valuable insight into the fundamental decomposition behavior of HE, but also enable a more complete understanding of the shock initiation response of high explosives after and during exposure to EM energy, which is imperative to ensure their safe use in weapon systems during storage, transport and deployment.

First Measurement of the Scale Anomaly in Dirac Semimetals

Michael Pettes
20210782ER

Project Description

The scale or conformal anomaly refers to the quantum many-body effect of the dependence of coupling 'constants' upon the distance or energy scale at which they are measured. It is called a quantum anomaly because it explicitly depends upon Planck's constant, and there is no such dependence upon scale in a purely classical setting, if the Hamiltonian is scale invariant, as for example it is in the case of massless or gapless fermions. Particular interest attaches to the scale anomaly because it tracks the response of a quantum system to external gravitational fields, or in General Relativity of quantum matter to the curvature of space and time. As there are very few experimental tests of quantum theory in General Relativity, the possibility of testing the scale anomaly in a controlled laboratory environment by a relatively small and inexpensive table-top experiment is essentially unique. This project will be the only laboratory measurement – even indirectly – of the scale anomaly, and a positive measurement will have far-reaching implications for quantum effects in gravitational fields or curved spacetime, in addition to establishing a new magneto-thermal measurement capability at Los Alamos National Laboratory.

Publications

Journal Articles

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

Pettes, M. T., A. Londono Calderon, R. Dhall, C. Ophus, Y. Wang, E. Dervishi-Whetham, H. S. Kang, C. Lee and J. Yoo. Visualizing Grain Statistics in MOCVD WSe through Four-Dimensional Scanning Transmission Electron Microscopy. 2022. *Nano Letters*. (LA-UR-21-30267 DOI: 10.1021/acs.nanolett.1c04315)

Presentation Slides

Parida, S., Y. Wang, H. Zhao, H. Htoon, T. Choudhury, J. Redwing, A. Dongare and M. T. Pettes. Mechanical Tuning of the Electronic and Vibrational Properties of Epitaxial MoS2 through Ion Beam Modification. Presented at *2021 MRS Fall Meeting & Exhibit*, Boston, Massachusetts, United States, 2021-11-29 - 2021-11-29. (LA-UR-21-31636)

Pettes, M. T. Towards control over 2D material properties through ion beam modification and analysis. Presented at *CINT 2021 Annual Meeting*, Online, New Mexico, United States, 2021-09-21 - 2021-09-21. (LA-UR-21-29318)

Pettes, M. T. Emergent Phenomena in van der Waals Materials: Advancements in Characterization. Presented at *Invited talk at University of Southern California*, Los Angeles, California, United States, 2021-05-28 - 2021-05-28. (LA-UR-21-31292)

Pettes, M. T. and A. B. Saxena. 20210782ER Progress FY21: First Measurement of the Scale Anomaly in Dirac Semimetals. . (LA-UR-21-30406)

Self-powered, low cost semiconductors for smart computation

Wanyi Nie
20210783ER

Project Description

This project aims to explore new smart computing devices to enable artificial intelligence coupled smart electronic network. By integrating new semi conducting materials to be investigated in this project, we will develop self-powered computer element that can be operated by ambient energy. This will allow for the network to perform computation tasks without the need of external power input. The outcome from this exploratory project will open up new opportunities for smart electronics like radiation sensor, computer networks coupled with artificial intelligence. These can be used to address Department of Energy/ National Nuclear Security Administration (DOE/NNSA) missions like smart nuclear material manufacturing, remote waste treatment. It will also provide future electronic technologies to address challenges in energy and information security missions.

Publications

Journal Articles

. G. D. *. J. K. L. *. F. D. *. S. A. *. L. S. G. *. L. F. *. N. W. *. B. J. *. Z. L. *. C. J. J. *. M. N. *. M. A. D. *. T. S. *. N. A. J. Lewis, S. G., S. G. Lewis, D. Ghosh, F. Liu, W. Nie, L. Zhou, J. J. Crochet, S. Tretiak, A. J. Neukirch and N. Moody. Cesium-Coated Halide Perovskites as a Photocathode Material: Modeling Insights. 2021. *The Journal of Physical Chemistry Letters*. **12 (27): 6269-6276. (LA-UR-21-24212 DOI: 10.1021/acs.jpclett.1c01412)

Mora Perez, C. A., D. Ghosh, O. Prezhdo, W. Nie, S. Tretiak and A. J. Neukirch. Point Defects in 2D Ruddlesden-Popper Perovskties Explored with ab initio Calculations. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-22-21646)

Shrestha, S., X. Li, H. Tsai, C. Hou, H. Huang, D. Ghosh, J. Shyue, L. Wang, S. Tretiak, X. Ma and W. Nie. Long carrier diffusion length in two-dimensional lead halide perovskite single crystals. Submitted to *CHEM*. (LA-UR-21-29516)

Tsai, H., D. Ghosh, E. Kinigstein, B. Dryzhakov, H. R. Driscoll, M. T. Owczarek, B. Hu, X. Zhang, S. Tretiak and W. Nie. Light Induced Structural Dynamics and the Charge Transport in Butylamine Lead Bromide Layered Perovskite Thin Films. Submitted to *Nature Materials*. (LA-UR-21-31869)

Tsai, H., H. Huang, J. D. Watt, C. Hou, J. Strzalka, J. Shyue, L. Wang and W. Nie. Cesium lead halide perovskite nanocrystals assembled in metal-organic frameworks for stable blue light emitting diodes. Submitted to *Advanced Materials*. (LA-UR-21-30401)

Presentation Slides

Nie, W. Low-dimensional Metal Halide Hybrid Perovskite Semiconductors for Light Emitting Devices. Presented at *Material Research Society, spring 2021*, Web meeting, New Mexico, United States, 2021-04-21 - 2021-04-27. (LA-UR-21-23773)

Accurate and Local Forces for Meso-Scale Methods

Ann Wills
20210786ER

Project Description

Models of materials behavior are crucial for all computer simulations performed in science and engineering. Rubber and steel, for example, behave very differently when under pressure. At the very small scales of quantum physics (nanometers = 1 billionth of a yard) we have rigorous mathematical equations (the Dirac and Schrodinger equations) that we can solve to understand materials properties. However, at the engineering scales (millimeter = 1 million times the quantum scale), we have to infer models and parameters from macroscopic studies, mostly experiments. There is a desire to bridge this scale gap using meso-scale methods in order to improve current macro-scale materials models. But meso-scale methods currently rely on expensive-to-calculate, *non-local* forces. Based on a few fundamental theorems and conjectures, we will investigate the possibility of creating a new method for calculating *local* forces. If such a method can be developed it would revolutionize our ability to perform meso-scale simulations and considerably improve our ability to create accurate materials models for use in engineering scale codes.

Publications

Journal Articles

Wills, A. E., S. Marrow and D. A. Rehn. Pathway to Accurate and Local Forces for Mesoscale Physics. Submitted to *Modelling and Simulation in Materials Science and Engineering*. (LA-UR-22-21704)

Supersonic dislocations? A key to unraveling material strength under extreme conditions.

Daniel Blaschke
20210826ER

Project Description

Computer simulations of materials under extreme pressure and high temperatures are needed to high precision by LANLs national security mission. As some of these regimes cannot be directly measured, we need a good first-principles understanding of the underlying physics of dislocations (line-defects) in metals. Currently used phenomenological strength models in contrast, lack predictability beyond regimes they have been calibrated to. This is the gap we aim to fill within this project.

Publications

Journal Articles

Blaschke, D., K. Q. Dang, S. J. Fensin and D. J. Luscher. Properties of accelerating edge dislocations in arbitrary slip systems with reflection symmetry. Submitted to *TBD*. (LA-UR-22-22567)

Dang, K. Q., D. Blaschke, S. J. Fensin and D. J. Luscher. Limiting velocities and transsonic dislocations in Mg. Submitted to *TBD*. (LA-UR-22-22557)

Presentation Slides

Blaschke, D., K. Q. Dang, S. J. Fensin, J. Chen, B. A. Szajewski and D. J. Luscher. Accelerating and supersonic dislocations in metals under extreme conditions. Presented at *TMS 2022 Annual Meeting & Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-02-27. (LA-UR-22-21620)

Using Earth's Magnetic Field for Battery Diagnostics

Benjamin Davis
20210827ER

Project Description

Batteries have become ubiquitous in everyday life with new applications being added every day. While battery usage is expected to drastically increase over the next 10 years, ensuring that the batteries are safe and reliable remains an outstanding issue. Many of the monitoring devices used for national security, particularly in the field, rely on these batteries and recent defects have resulted in explosions and catastrophic failure of the batteries. In this work, we will make a new type of battery diagnostic device leveraging nuclear magnetic resonance spectroscopy (NMR). This is the same technology used by medical Magnetic Resonance Imaging (MRI) instruments. In a similar manner to MRI, our device will be able to non-invasively examine the chemical composition of a sample. However, unlike MRI, which used very large magnetic fields, we propose to use Earth's magnetic field, which is freely available through-out the world. Once the instrument is built and optimized, we will test the feasibility of detecting defects in commercially available batteries.

Publications

Journal Articles

Kaseman, D., R. J. Batrice and R. F. Williams. Detection of Natural Abundance 13C J-couplings at Earth's Magnetic Field for Spin System Differentiation of Small Organic Molecules. Submitted to *Journal of the American Chemical Society*. (LA-UR-22-22496)

Ion Beam Synthesis of Layer-Tunable, Transfer-Free and Chemically Doped Graphene Films on Arbitrary Substrates

Yongqiang Wang
20210867ER

Project Description

To exploit graphene as a key electronic material, with its unique two-dimensional (2-D) hexagonal lattice structure and extraordinary physical properties, in nanoelectronics and flexible electronic devices applications, direct synthesis of layer-tunable graphene, independent of device substrates along with desired chemical doping characteristics, is needed. The current process involves separate growth, transfer, and doping steps. This project attempts to explore a novel ion beam-based approach that lets one synthesize doped layer-tunable graphene films on technologically-relevant substrates in a single step. The innovation is based on a large solubility difference of carbon (or boron(B)/nitrogen(N) as dopants) in different metals, e.g. a copper-nickel (Cu-Ni) bilayer smart Janus structure. During the bi-metal layer alloying process, while annealing after implantation , the pre-implanted carbon atoms (B or N dopants) are forced to precipitate onto the substrate to form a graphene film already positive- or negative-type doped due to their solubility differences between Cu and Ni. Since ion implantation is a mature technology in microelectronics industry, success of this project has potential to expedite graphene applications in versatile device applications. The materials by design knowledge gained through this project will also benefit in synthesizing other 2-D quantum material structures with desired functionalities and performance characteristics.

Utilizing Crystalline Sponges to Perform Single Crystal X-ray Determination on Trace Amounts of Actinium Compounds

Brian Scott
20180128ER

Project Description

Actinium shows great promise as a cancer radioimmunotherapy agent. However, its scarcity has hindered chemical structure characterization with X-rays. Chemical structure is vital to understanding how actinium will behave in biological systems and also for designing therapeutic agents. This work will develop techniques to perform X-ray single crystal characterization using trace amounts of actinium absorbed into porous crystals. These porous crystals, known as metal-organic-frameworks (MOF's), are composed of metal centers linked together with organic molecules to form a three-dimensional structure with open pores. Microgram quantites of actinium are not sufficient to grow crystals for X-ray studies, but do provide ample material for an actinium-MOF crystal that can be used for X-ray structure determination. An MOF crystal large enough for X-ray studies can absorb micrograms of actinium into its pores. An X-ray crystal structure of the actinium containing MOF crystal will yield the structure of the MOF and the absorbed actinium species. Besides informing radioimmunotherapy development using actinium, this technique could also be used to determine chemical structure of trace amounts of chemical weapons agents, explosives, and other actinides and molecules of importance to national security.

Technical Outcomes

We identified and structurally characterized a stable metal organic framework (MOF) crystal with a uranyl ion as guest. This system is a model for actinide interactions with minerals, and also a potential nuclear waste form. A series of MOF's with other metal complexes were identified, but could not be structurally characterized. These systems provide a series of MOF-metal complex systems that provide a foundation for future studies in this class of materials.

Publications

Journal Articles

Klamm, B. E., K. Bhardwaj, S. M. Greer, H. D. Root, S. Sharma, C. J. Windorff, M. M. MacInnes, S. H. Carpenter, T. E. Albrecht-Schonzart, B. L. Scott, B. Stein, S. A. Kozimor and A. Tondreau. Caging Plutonium. Submitted to *Inorganic Chemistry*. (LA-UR-21-28031)

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

*Knapp, J. G., X. Zhang, T. Elkin, L. E. Wolfsberg, S. L. Hanna, F. A. Son, B. L. Scott and O. K. Farha. Single crystal structure and photocatalytic behavior of grafted uranyl on the Zr-node of a pyrene-based metal–organic framework. 2020. *CrystEngComm*. **22** (11): 2097-2102. (LA-UR-21-22931 DOI: 10.1039/C9CE02034A)

Reports

Scott, B. L., G. S. Goff, D. A. Yarotski, P. C. Dowden, L. E. Wolfsberg and G. Rodriguez. Experimental Signatures for Dynamic Plutonium Hydriding. Unpublished report. (LA-UR-19-20942)

Presentation Slides

Elkin, T. Development of novel MOFs for (CWA) emerging threats. Presented at *IMS Rapid response workshop*, Evanston, Illinois, United States, 2019-09-10 - 2019-09-12. (LA-UR-19-29055)

Root, H. D. Applications of Porphyrinoid Macrocycles in Molecular Sensing and f-Element Coordination. . (LA-UR-20-24682)

Electronic Structure of Putative Topological Kondo Insulators

Mun Chan
20180137ER

Project Description

We will develop the capability to study electronic and magnetic properties of materials under simultaneous ultra-high pressures and high-magnetic fields. This will be applied to the study of topologically correlated electron materials, a field that promises significant technological implications, including ultra-fast quantum computation and spintronics. It is of vital importance to the Los Alamos mission to understand the properties of materials under pressure. Crystalline properties are routinely tracked with x-rays. Our new experimental capability will allow for a determination of the electronic properties. This will foster new collaborations at the high-magnetic field laboratory at the Laboratory.

Technical Outcomes

We synthesized high quality crystals of Kondo insulators which have been predicted to host topological band-structures. These crystals were studied with large pulsed magnetic fields to reveal their electronic properties. We ascertained that the studied materials were not topological, however we measured a magnetic field driven quantum critical point for the first time in these materials. We developed a prototype diamond anvil cell capable of achieving high-pressures in a pulsed magnet environment.

Publications

Journal Articles

Chan, M. K., T. Sarkar, J. Higgins, P. Mandal, N. Poniatowski and R. Greene. Strange Metallic Transport in the Antiferromagnetic Regime of Electron Doped Cuprates. Submitted to *Physical Review X*. (LA-UR-20-24641)

*Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. F. S. Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Nature Communications*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

Visualizing Nanoscale Spatio-Temporal Dynamics in Single Quantum Systems

Peter Goodwin
20180189ER

Project Description

This project is responsive to the Laboratory mission in the Materials for the Future Focus area in that it strives, through the development of novel characterization methods for the visualization of excited state dynamics in nanoengineered structures, for 'linking across length and time scales … to achieve a multi-scale understanding, and ultimately control, of materials structure, dynamics and function.' These studies will uncover detailed aspects of quantum dot (QD) interparticle interactions that will be relevant toward designing and improving QD optoelectronic devices, displays, solar cells, biological labels, and other technologies, and will enable the discovery of new properties and unanticipated applications and devices involving QDs. These studies will also reveal features of electronic energy interactions unique to QDs and other nanoparticles, as well as features common to molecular systems in which excited state electronic interactions are important, such as organic molecule Förster resonance energy transfer (FRET), conjugated polymers, and biological photosynthetic complexes. Finally, this research will introduce new experimental methods and capabilities that can be exploited to investigate a wide variety of molecular and nanoscale systems, in which multiple emitters cluster, aggregate, or associate to transport electronic energy in a manner that is greater than the sum of its parts.

Technical Outcomes

This project developed methods for the measurement of fluorescence dynamics in nanoscale systems to enable visualization of energy transport in the same: 1) super-resolution optical imaging with sub-nanosecond time resolution; 2) polarization-resolved super-resolution imaging to elucidate electronic dipole orientations in nanoscale systems. The first was achieved using a four-element detector, time-correlated single-photon counting, and pulsed laser excitation. The second utilized wide-field polarization- and spectrally-resolved imaging.

Both approaches were used to characterize small clusters of nanocrystal quantum dots.

Publications

Journal Articles

*Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. Van Orden. Super-resolution photoluminescence lifetime and intensity mapping of interacting CdSe/CdS quantum dots. 2020. *Applied Physics Letters*. **116** (2): 021103. (LA-UR-19-30441 DOI: 10.1063/1.5132563)

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. Van Orden. Single Molecule Localization With Four Avalanche Photodiode Detectors. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-20171)

. D. M. K. *. G. M. P. *. W. J. H. *. V. O. A. K. *. G. P. M. Ryan, D. P., D. P. Ryan, J. H. Werner and P. M. Goodwin. A gain series method for accurate EMCCD calibration. 2021. *Scientific Reports*. **11 (1): 18348. (LA-UR-21-24123 DOI: 10.1038/s41598-021-97759-6)

Ryan, D. P., M. K. Dunlap, J. A. Hollingsworth, S. Majumder, J. H. Werner, M. P. Gelfand, A. K. Van Orden and P. M. Goodwin. Collective optical behavior from coupled quantum dots visualized by spectral- and polarization-resolved superresolution microscopy. Submitted to *Nature Nanotechnology*. (LA-UR-22-20078)

Ryan, D. P., M. K. Dunlap, J. A. Hollingsworth, S. Majumder, M. Gelfand, J. H. Werner, A. K. Van Orden and P. M. Goodwin. Quantum dot clusters visualized by polarization- and wavelength-resolved nanoscopy. Submitted to *Nature Nanotechnology*. (LA-UR-21-28192)

Ryan, D. P., M. K. Dunlap, S. Majumder, C. J. Sheehan, J. H. Werner, J. A. Hollingsworth, M. P. Gelfand and A. K. Van Orden. Dual-color super-resolution imaging for FRET measurements: Energy transfer among donor/acceptor pairs of quantum dots. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-20052)

*Ryan, D. P., M. K. Dunlap, S. Majumder, J. H. Werner, J. A. Hollingsworth, M. P. Gelfand, A. Van Orden and P. M. Goodwin. A framework for quantitative analysis of spectral data in two channels. 2020. *Applied Physics Letters*. **117** (2): 024101. (LA-UR-20-23550 DOI: 10.1063/5.0013998)

*Ryan, D. P., P. M. Goodwin, C. J. Sheehan, K. J. Whitcomb, M. P. Gelfand and A. Van Orden. Mapping Emission from Clusters of CdSe/ZnS Nanoparticles. 2018. *The Journal of Physical Chemistry C*. **122** (7): 4046-4053. (LA-UR-18-20821 DOI: 10.1021/acs.jpcc.7b10924)

Ryan, D. P., P. M. Goodwin, J. H. Werner, M. K. Dunlap, A. K. Van Orden and M. P. Gelfand. From Noise to Harmony: Calibration Methods for Electron Multiplying CCD Cameras. Submitted to *Optics Express*. (LA-UR-20-27551)

Presentation Slides

Dunlap, M. K. Time-resolved Super-resolution Microscopy Studies of Quantum Dot Aggregates. . (LA-UR-21-20441)

Dunlap, M. K. Time-Resolved Super-Resolution Microscopy Studies of Quantum Dot Clusters. . (LA-UR-21-21336)

Dunlap, M. K. Time-resolved super-resolution microscopy studies of quantum dot clusters. . (LA-UR-21-22308)

Dunlap, M. K. Quantum Dot Studies with Time-Resolved Super-Resolution Microscopy. . (LA-UR-21-26255)

Goodwin, P. M., J. H. Werner, J. A. Hollingsworth, M. K. Dunlap, D. P. Ryan, S. Majumder, A. Van Orden and M. P. Gelfand. 20180189ER Visualizing Nanoscale Spatio-Temporal Dynamics in Single Quantum Systems. . (LA-UR-20-23772)

Ryan, D. P. Energy Flow through Quantum Dot Networks. . (LA-UR-18-25130)

Ryan, D. P. Exploring Interactions among Nanocrystals with Multidimensional Nanoscopy. . (LA-UR-21-29673)

Ryan, D. P., A. K. Van Orden, J. A. Hollingsworth, M. K. Dunlap, J. H. Werner, P. M. Goodwin, C. J. Sheehan, S. Majumder and M. P. Gelfand. Camera-based single-particle orientation imaging of quantum dots. Presented at *SPIE Photonics West: BiOS*, San Francisco, California, United States, 2021-03-06 - 2021-03-11. (LA-UR-21-21334)

Ryan, D. P., M. K. Dunlap, P. M. Goodwin, J. H. Werner, J. A. Hollingsworth, S. Majumder, C. J. Sheehan, A. K. Van Orden and M. Gelfand. Dual-color Super-resolution Imaging of Quantum Dot Clusters. Presented at *SPIE Photonic West 2020*, San Francisco, California, United States, 2020-01-31 - 2020-02-06. (LA-UR-20-20728)

Ryan, D. P., M. K. Dunlap, S. Majumder, C. J. Sheehan, J. A. Hollingsworth, M. P. Gelfand, P. M. Goodwin and A. K. Van Orden. Super-resolution Imaging for Energy Transfer: Collective behavior from interacting quantum dots. Presented at *American Chemical Society Annual Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22627)

Ryan, D. P., P. M. Goodwin, J. H. Werner, C. J. Sheehan, J. A. Hollingsworth, S. Majumder, M. K. Dunlap, A. Van Orden and M. Gelfand. Energy Transfer Through Networks of CdSe/CdS Nanoparticles. Presented at *Gordon Research Conference on Colloidal Semiconductor Nanocrystals*, Smithfield, Rhode Island, United States, 2018-07-15 - 2018-07-20. (LA-UR-18-26595)

Werner, J. H. and M. Dunlap. Quantum dot studies with time-resolved super-resolution microscopy. Presented at *Idaho State University Physics Colloquium*, pocatello, Idaho, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30952)

Posters

Abdollah-nia, F., M. K. Dunlap, J. Gann, D. P. Ryan, P. M. Goodwin, J. A. Hollingsworth, Y. Chen, J. S. Martinez, M. Gelfand and A. Van Orden. Single Molecule Experiments in the Van Orden Resarch Group. Presented at *Colorado State University Chemistry Graduate Student Recruiting Weekend*, Fort Collins, Colorado, United States, 2019-02-15 - 2019-02-15. (LA-UR-19-21376)

Dunlap, M. K., A. K. Van Orden and J. Gahn. Single Molecule Studies in the Van Orden Group. . (LA-UR-21-21337)

Dunlap, M. K., D. P. Ryan, J. H. Werner, J. A. Hollingsworth, M. Gelfand, A. Van Orden and P. M. Goodwin. A Lifetime Imaging Super-Resolution Microscope. Presented at *ACS Spring 2019 National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-03. (LA-UR-19-23084)

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, J. A. Hollingsworth, M. Gelfand and A. Van Orden. Sub-Nanosecond Superresolution Imaging of Energy Transfer in CdSe/CdS Quantum Dot Clusters. . (LA-UR-19-24114)

Dunlap, M., D. P. Ryan, M. Gelfand and P. M. Goodwin. Quantum Dot Localization with Time Resolved Super-Resolution Tracking Microscopy. Presented at *Annual Meeting of the APS Four Corners Section*, Fort Collins, New Mexico, United States, 2017-10-20 - 2017-10-21. (LA-UR-17-29934)

Dunlap, M., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. K. Van Orden. Characterizing the Spatial Information of a Superresolution Fluorescence Lifetime Imaging Microscope. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28791)

Ryan, D. P., M. Dunlap, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand, A. K. Van Orden and C. J. Sheehan. Energy Transfer Through Networks of CdSe/CdS Nanoparticles. Presented at *Gordon Research Conference on Colloidal Semiconductor Nanocrystals*, Smithfield, Rhode Island, United States, 2018-07-14 - 2018-07-20. (LA-UR-18-25908)

Ryan, D. P., S. Majumder, J. A. Hollingsworth, J. H. Werner, P. M. Goodwin, A. K. Van Orden, M. K. Dunlap and M. P. Gelfand. Emission Dynamics from Clusters of Quantum Dots. Presented at *CINT Annual User Meeting*, Santa Fe,

New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29347)

Ryan, D. P., S. Majumder, J. A. Hollingsworth, P. M. Goodwin, J. H. Werner, M. K. Dunlap, A. K. Van Orden and M. P. Gelfand. Super-resolution Orientation Imaging: A Microscopy Method for Measuring Structure in Biological Samples. Presented at *Biophysical Society Meeting*, San Francisco, California, United States, 2020-02-14 - 2020-02-19. (LA-UR-20-21373)

Improved Biologically Friendly Polymer Drag Reducers From Novel Architectures

Paul Welch
20180220ER

Project Description

The research described in this proposal will directly address the Objective Capability Area of Mitigating Impacts of Global Energy Demand Growth called out in the Los Alamos Energy Security Strategy. Specifically, we will address the objective of "Integrating multi-scale measurements, modeling,and uncertainty quantification to validate predictions to support decisions and investments in energy systems with a goal of anticipating risks, disruptions, impacts, and consequences." This project will produce a series of polymers designed to reduce drag in aqueous flows. The project will study the molecular physics involved in the polymer interactions in turbulent environments over a range of length and time scales using a novel combination of experimental and modeling techniques. Success in this project will produce new insight into the importance of molecular architecture in drag reduction, facilitating the design of new materials. In particular, we will learn: 1) whether intrinsically multi-time scale materials perform better in typical drag reduction applications; 2) how best to design the distribution of molecular time scales to optimally impact realistic flow fields; and 3) the biologically friendly chemical architectures that most likely satisfy that distribution.

Technical Outcomes

The primary technical findings are that: i) branched polyelectrolytes display chimeric characteristics as a function of molecular architecture and environment; ii) in porous media, drag reducing polymers usually lead to drag enhancement; iii) surprisingly, turbulence may be realized in microfluidic devices. Moreover, the team wrote new simulation codes, devised new synthetic routes to novel copolymers, and constructed three experimental testbeds that mimic application environments. These tools position the Laboratory for studies of the energy-water nexus.

Publications

Journal Articles

J. Welch, P. M. and C. F. Welch. Calculating Dendrimer Titration Curves through Quantum Annealing. Submitted to *ACS Macro Letters*. (LA-UR-19-27637)

Posters

Schmidt, J. G., C. Schein, D. Beasley, M. Braun and D. Weaver. Stabilized PCP-Consensus Peptides for Flavi- and Alphavirus Vaccines and Therapies. Presented at *CBS&T*, Cincinnatti, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-30920)

Ultrafast X-ray Imaging Using Slow, Visible Cameras

Pamela Bowlan
20180242ER

Project Description

New bright sources of femtosecond (10-15 seconds) X-ray pulses are revolutionizing materials science giving atomic-scale snap shots of how materials behave in extreme conditions like high pressure or temperature. A major impediment in these experiments are the detectors which have temporal resolutions up to six orders of magnitude slower than the X-ray pulses, smearing out the dynamics being studied, and making it challenging to even diagnose the X-ray source. Future X-ray Free Electron Lasers, aimed to directly address DOE/NNSA mission goals like manufacturing science or dynamics in explosives, will use even higher X-ray photon energies and operate at higher X-ray pulse frequencies, for which no detector exists. Our work offers a novel, potentially transformative solution, where interacting an X-ray and visible light pulse in the right medium encodes the X-ray pulse's spatial and temporal information (i.e., the X-ray image and its femtosecond temporal evolution) in the visible light, making it possible to measure femtosecond time resolved X-ray images with standard visible cameras. This technology will both improve the capabilities at current DOE X-ray sources, and also help to motivate and build new sources optimized specifically for NNSA mission-relevant applications.

Technical Outcomes

The project successfully demonstrated that high frequency femtosecond pulses can be measured by encoding their pulse shape in a visible nonlinear optical signal. This method was demonstrated at a Free Electron Laser. This method has the potential to become an online diagnostic at Free Electron Lasers.

Publications

Journal Articles

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Measuring an ultrashort pulse in a slowly responding, absorbing medium. Submitted to *Optics Express*. (LA-UR-20-30027)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Response Letter. Submitted to *Optics Express*. (LA-UR-21-21553)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Supplemental Information for Measuring an ultrashort, ultraviolet pulse in a slowly responding, absorbing medium. Submitted to *Optics Express*. (LA-UR-21-21552)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. Trebino and P. R. Bowlan. Measuring an ultrashort, ultraviolet pulse in a slowly responding, absorbing medium. Submitted to *Optics Express*. (LA-UR-21-21551)

Jones, T. N., W. K. Peters, A. V. Efimov, R. L. Sandberg, D. A. Yarotski, R. P. Trebino and P. R. Bowlan. Measuring an ultraviolet ultrashort pulse by encoding it in a near-infrared nonlinear-optical signal pulse. Submitted to *OSA Continuum*. (LA-UR-20-24221)

Jones, T. N., W. K. Peters, A. V. Efimov, R. L. Sandberg, D. A. Yarotski, R. P. Trebino and P. R. Bowlan. Encoding the complete electric field of an ultraviolet ultrashort laser pulse in a near-infrared nonlinear-optical signal. Submitted to *Optics Express*. (LA-UR-20-26396)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, R. Trebino, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. All-optical single shot complete electric field measurement of extreme ultraviolet free electron laser pulses. Submitted to *Nature Photonics*. (LA-UR-20-27156)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, R. Trebino, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. All-optical single shot complete electric field measurement of extreme ultraviolet free electron laser pulses. Submitted to *Optica*. (LA-UR-21-20565)

Trebino, R., R. Jafari, S. Akturk, P. Piksarv, P. R. Bowlan, H. Valtna-Lukner, P. Saari, Z. Guang, P. Zhu and G. Steinmeyer. Tutorial: The Measurement of Ultrashort Laser Pulses. Submitted to *Journal of Applied Physics*. (LA-UR-20-24953)

Reports

Bowlan, P. R. Ultrafast Control of Material Properties though Core Electrons. Unpublished report. (LA-UR-18-21644)

Presentation Slides

Bowlan, P. R. Detecting femtosecond x-ray pulses with slow visible cameras. Presented at *Internal C-division seminar*, Los Alamos, New Mexico, United States, 2021-06-16 - 2021-06-16. (LA-UR-21-25676)

Bowlan, P. R., M. S. Powell and S. D. Mcgrane. Ultrafast mid-IR measurements during shock. Presented at *Shocked chemistry LDRD review*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-06. (LA-UR-18-20743)

Bowlan, P. R., T. N. Jones and R. L. Sandberg. Travis' LANL Experience. Presented at *Meeting with Rick Trebino's research group (talk to be given by Travis Jones)*, Atlanta, Georgia, United States, 2019-01-15 - 2019-01-15. (LA-UR-19-20252)

Jones, T. N. Complete Temporal Measurement of Low-Intensity and High-Frequency Ultrashort-Presentation. . (LA-UR-20-29379)

Jones, T. N. Job Talk. . (LA-UR-21-24869)

Jones, T. N., W. K. Peters, A. V. Efimov, D. A. Yarotski, R. L. Sandberg, R. Trebino and P. R. Bowlan. Measuring ultraviolet, femtosecond pulses in a medium with a slow response. Presented at *Conference on Lasers and Electro-Optics (CLEO)*, San Jose, California, United States, 2020-05-10 - 2020-05-15. (LA-UR-20-23467)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, R. Trebino, R. L. Sandberg, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. Single-shot Measurement of Extreme Ultraviolet Free Electron Laser Pulses. Presented at *Conference on Lasers and Electro-optics*, San Joase, California, United States, 2020-05-11 - 2020-05-11. (LA-UR-20-23468)

Peters, W. K. and P. R. Bowlan. Single-shot Measurement of Extreme Ultraviolet Free Electron Laser Pulses And a few other measurements using ultrafast, short-wavelength lasers. . (LA-UR-20-25717)

Posters

Jones, T. N., W. K. Peters, R. L. Sandberg and P. R. Bowlan. Measuring Femtosecond Extreme-Ultraviolet Pulses With Slow Visible Cameras. Presented at *LANL Annual Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27709)

Peters, W. K., T. N. Jones, A. V. Efimov, E. Pedersoli, L. Foglia, R. Mincigrucci, I. Nikolov, M. Danailov, F. Capotondi, F. Bencivenga and P. R. Bowlan. Single-shot, all-optical complete electric field measurement of extreme ultraviolet free electron laser pulses. Presented at *2020 Virtual SSRL/ LCLS Users' Meeting*, Menlo Park, California, United States, 2020-09-28 - 2020-10-09. (LA-UR-20-27432)

Peters, W. K., T. N. Jones, P. R. Bowlan and R. L. Sandberg. Nonlinear Optics with Ionizing Radiation and Ultrafast Lasers: Progress Toward Measuring the Complete Electric Field of XFEL Pulses. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28443)

Tuning Functionality via Dimensionality in 4f-Based Nanowires

Priscila Rosa
20190076ER

Project Description

This project directly addresses a basic research need for energy and security relevant technology by providing the science required to discover, understand and ultimately control nanostructured forms of matter. Our approach is enabled by the ability to exploit low-dimensional correlated systems to tune functionality. Not only addressing a fundamental problem that is unexplored experimentally, this project also brings a new capability of probing 4f-based nanowires that will enable understanding and control of new materials and new physics that may emerge in the future.

Technical Outcomes

The goal of this project is to experimentally probe the unexplored effects of dimensionality in correlated intermetallic low-dimensional materials, including nanowires, via electrical and magnetic measurements. The team successfully investigated the effects of dimensionality in three different classes of f-electron low-dimensional materials. In addition, our team established a well-grounded experimental framework necessary to reliably manipulate and electrically probe nanowires. This includes fabrication via e-beam lithography or focused-ion beam combined with platinum deposition.

Publications

Journal Articles

Avers, K. E., P. A. Maksimov, P. Rosa, S. M. Thomas, J. D. Thompson, W. P. Halperin, R. Movshovich and A. L. Chernyshev. Fingerprinting Triangular-Lattice Antiferromagnet by Excitation Gaps. Submitted to *Physical Review B*. (LA-UR-21-25027)

Ronning, F., S. Lee, S. Seo, K. E. Avers, S. M. Thomas, R. Movshovich, J. D. Thompson, P. Rosa, E. D. Bauer and T. Asaba. Physical properties of quasi-one-dimensional YbFe5P3. Submitted to *Physical Review B*. (LA-UR-21-28341)

Shockwave Metamaterials: Harnessing Structural Hierarchy for Tailorable Dynamic Response

Dana Dattelbaum
20190084ER

Project Description

Structural materials that function extensively as structural supports and protective components in aerospace and military applications are poised for transformational improvements through an ability to control structure with the advent of additive manufacturing. To date, these advances have been almost entirely related to tailorable mechanical response with only a limited number of studies interrogating the performance of these materials under the high strain rate-deformation, extreme conditions relevant to conventional and nuclear weapons environments. This project aims to lead the development of novel materials through dynamic characterization, materials modeling at high strain rates, along with the high resolution printing capabilities in order to understand the behavior of additively manufactured (AM) materials and their ability to tailor shockwave propagation offering a new class of materials for future stockpile applications.

Technical Outcomes

Interface-dominated structures show promise for dissipating shock wave energy through two effects: viscoplastic deformation and edge-release wave interactions on relevant timescales. Analysis has shown high localization of dissipation at the interfaces. The sound velocity at pressure, and compressibility dictate the shock and rarefaction wave speeds that result in a "ringing-down" of the shock stress. A new topological optimization approach was developed within Abaqus Explicit for optimizing shockwave dissipation which is the first of its kind.

Publications

Journal Articles

*Dattelbaum, D. M., A. Ionita, B. M. Patterson, B. A. Branch and L. Kuettner. Shockwave dissipation by interface-dominated porous structures. 2020. *AIP Advances*. **10** (7): 75016. (LA-UR-20-23537 DOI: 10.1063/5.0015179)

Dattelbaum, D. M., B. Branch, A. Ionita, B. M. Patterson and L. A. Kuettner. Shockwave interactions with additively-manufactured polymer structures. Submitted to *AIP Conference Proceedings*. (LA-UR-19-27099)

Ionita, A., D. M. Dattelbaum and B. M. Patterson. Topological Derivative-based Topological Optimization for Shockwave Energy Dissipation Materials. Submitted to *Structural and Multidisciplinary Optimization*. (LA-UR-21-28821)

Presentation Slides

Dattelbaum, D. M., B. Branch, A. Ionita, B. M. Patterson and L. A. Kuettner. Shockwave interactions with additively-manufactured polymer structures (U). Presented at *2019 American Physical Society Shock Compression of Condensed Matter Topical Group meeting*, Portland, Oregon, United States, 2019-06-16 - 2019-06-22. (LA-UR-19-25436)

Air-Buoyant Vessel

Miles Beaux
20190119ER

Project Description

Remote sensing payloads, suspended from weather balloons for nonproliferation and treaty verification (as well as other surveillance applications), represent a potentially cheaper alternative to orbital satellite payloads. However, these ballooning applications face challenges such as the ever-increasing cost and decreasing supply of helium, the difficulty and cost of transporting helium, and the tendency of payloads to come down in undesirable locations which can be problematic for sensitive surveillance applications. This project aims to produce an air buoyant vacuum vessel (aka a vacuum balloon) as a helium-free alternative to weather balloons for suborbital atmospheric payload deployment. By utilizing a vacuum vessel filled with "nothing" instead of helium, it is expected that more permanent payload deployment can be achieved while greatly reducing the cost and providing better control over targeted location decent. This will be accomplished by developing ultra-light weight super-strong materials to meet the stringent engineering requirements for an air buoyant solid structure to be viable.

Technical Outcomes

Fifteen grams of helical fibers were produced and composited with aerogel/cryogel materials, and the resulting mechanical advantage demonstrated. The optimal vacuum sealing density of aerogel/cryogel materials was isolated, and predictions related thereto confirmed. Hemispherical shells of material forming vacuum vessels were produced, tested, and imaged. The ability of these vacuum vessel to hold vacuum was verified, and a capabilities for producing an air-buoyant prototype established. Production of air-buoyant prototype still incomplete.

Publications

Journal Articles

I. Beaux, M. F., J. L. Hass, C. J. Hanson, S. L. Edwards, A. S. Edgar, D. R. Vodnik, B. L. Bennett, V. P. Siller, L. A. Kuettner, B. M. Patterson and C. E. Hamilton. Approaching Air Buoyancy in Aero/Cryogel Vacuum Vessels. Submitted to *Polymers*. (LA-UR-21-31651)

Presentation Slides

Hanson, C. J., S. L. Edwards and C. E. Hamilton. Additive Manufacturing and Novel Drying Methods Increase Accessibility and Decrease Integration Costs for Polyimide Aerogels. Presented at *5th Cross JOWOG on Additive Manufacturing*, Livermore, California, United States, 2020-01-27 - 2020-01-27. (LA-CP-20-20038)

Other

Ambrosiano, N. W. and M. F. I. Beaux. Balloon protype images. Audio/Visual. (LA-UR-20-27447)

Strongly Interacting Polariton Condensates at Room Temperature

Jinkyoung Yoo
20190224ER

Project Description

Quantum information science and technology will bring disruptive methods of information security, such as quantum computers powerful enough to break current encryption codes and quantum cryptography to prevent eavesdropping. However, the future is speculative because of the absence of suitable physical constituents for quantum information carriers. Current candidates for quantum information carriers do not fulfill the requirements of scalability, controllability, and robustness concurrently. Moreover, a few promising candidates require huge energy consumption due to quantum behaviors at cryogenic temperatures. This project aims at realizing robust and controllable quantum information carriers at room temperature in large scale. The physical constituents of the information carriers are interacting polariton condensates. Interacting polariton condensates will be made in semiconductor micro/nanocavity arrays embedding atomically thin quantum emitters. Interactions between polariton condensates can be controlled by external inputs. Thus, interacting polariton condensates can be used for computation. The system will be scalable due to the solid-state semiconductor platform -- a marked advantage over existing electronic systems. Additionally, polariton condensates are stable at room temperature. The expected deliverables will be breakthroughs in realization and deployment of quantum information systems.

Technical Outcomes

The project's goals were fabrication and characterization of cavity arrays embedding atomically thin nanomaterial. The team successfully fabricated high-quality and crystalline cavity arrays to study quantum fluid states. The fabricated cavity arrays showed a specific light-matter interacting behavior as desired. During the project execution, the team developed an approach to prepare material architectures composed of incommensurate materials. The approach is considered as a smart way to manufacture semiconductor devices for flexible applications and advanced nanodevices.

Publications

Journal Articles

*Jeong, J., Q. Wang, J. Cha, D. K. Jin, D. H. Shing, S. Kwon, B. K. Kang, J. H. Jang, W. S. Yang, Y. S. Choi, J. Yoo, J. K. Kim, C. Lee, S. W. Lee, A. Zakhidov, S. Hong, M. J. Kim and Y. J. Hong. Remote heteroepitaxy of GaN microrod heterostructures for deformable light-emitting diodes and wafer recycle. 2020. *Science Advances*. **6** (23): eaaz5180. (LA-UR-19-29399 DOI: 10.1126/sciadv.aaz5180)

Kim, Y., J. D. Watt, X. Ma, T. Ahmed, S. Kim, K. Kang, T. S. Luk, Y. J. Hong and J. Yoo. Fabrication of a microcavity prepared by remote epitaxy over monolayer molybdenum disulfide. Submitted to *Science Advances*. (LA-UR-21-28942)

*Kim, Y., T. Kim, J. Lee, Y. S. Choi, J. Moon, S. Y. Park, T. H. Lee, H. K. Park, S. A. Lee, M. S. Kwon, H. Byun, J. Lee, M. Lee, B. H. Hong and H. W. Jang. Tailored Graphene Micropatterns by Wafer-Scale Direct Transfer for Flexible Chemical Sensor Platform. 2020. *Advanced Materials*. 2004827. (LA-UR-20-29018 DOI: 10.1002/adma.202004827)

Wang, X., Y. Kim, J. K. S. Baldwin, A. C. Jones, J. Jeong, K. T. Kang, A. Chen and J. Yoo. Enhanced van der Waals epitaxy of germanium by out-of-plane dipole moment induced from transferred graphene on TiN/AlN multilayers. Submitted to *Journal of Applied Physics*. (LA-UR-21-27662)

Reports

Dervishi-Whetham, E. and J. Yoo. Recyclable graphene sheets as a growth template for crystalline ZnO nanowires. Unpublished report. (LA-UR-21-24375)

Presentation Slides

Kim, Y. Direct Polymer Curing Transfer &Surface Modification of 2D Materials for Flexible Electronics. Presented at *Seminar at Brookhaven National Laboratory*, Online, New Mexico, United States, 2021-06-11 - 2021-06-11. (LA-UR-21-25450)

Kim, Y., D. Kim, E. L. Auchter, J. Marquez, R. M. Tutchton, N. Li, T. S. Luk, E. Dervishi-Whetham, Y. Kim, J. Zhu and J. Yoo. Recycling of Two-Dimensional Materials for van

der Waals and Remote Epitaxy. Presented at *2021 MRS Spring*, Online, New Mexico, United States, 2021-04-17 - 2021-04-23. (LA-UR-21-23783)

Kim, Y., S. Swarnadeep, T. Ahmed, J. Jeong, S. Choi, Y. J. Hong, H. W. Jang, W. S. Yang and J. Yoo. Van der Waals epitaxy of germanium on multi-layer graphene/h-BN stacks: Limitation of screening out-of-plane dipole moment. Presented at *2020 MRS Virtual Spring/Fall meeting*, Online, New Mexico, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-29017)

Kim, Y., T. Kim, J. Lee, Y. S. Choi, J. Moon, S. Y. Park, T. H. Lee, H. K. Park, S. A. Lee, M. S. Kwon, H. Byun, J. Lee, M. Lee, B. H. Hong and H. W. Jang. Tailored Graphene Micropatterns by Wafer-Scale Direct Transfer for Flexible Chemical Sensor Platform. Presented at *2021 MRS Spring*, Online, New Mexico, United States, 2021-04-17 - 2021-04-23. (LA-UR-21-23784)

Yoo, J. Two-dimensional Materials Research at LANL. . (LA-UR-19-27080)

Yoo, J. Multi-dimensional van der Waals heterostructures. Presented at *31st Rio Grande Symposium on Advanced Materials*, Albuquerque, New Mexico, United States, 2019-09-16 - 2019-09-16. (LA-UR-19-29194)

Yoo, J. 2D/3D van der Waals heterostructures. Presented at *2019 Materials Research Society Fall Meeting*, Boston, Massachusetts, United States, 2019-12-02 - 2019-12-02. (LA-UR-19-31957)

Yoo, J. Nucleation control in van der Waals epitaxy. Presented at *2020 Materials Research Society Spring/Fall virtual meeting*, Boston, Massachusetts, United States, 2020-11-29 - 2020-11-29. (LA-UR-20-29297)

Yoo, J. Hybrid van der Waals heterostructures for quantum materials research. Presented at *2021 Korean Physical Society Spring Meeting*, Online, Korea, South, 2021-04-21 - 2021-04-23. (LA-UR-21-23782)

Yoo, J. Multi-dimensional nanomaterials for devices and QIS. . (LA-UR-21-24882)

Yoo, J. Realization of transition metal dichalcogenide embedding microcavity via remote epitaxy. Presented at *Epitaxy on two-dimensional materials*, Boston, Massachusetts, United States, 2021-06-30 - 2021-06-30. (LA-UR-21-26254)

Yoo, J. Multi-dimensional heterostructures prepared by recent epitaxy techniques. . (LA-UR-21-30769)

Posters

Yoo, J. Semiconductor Nano-heterostructures Research at CINT. . (LA-UR-19-24208)

Wavelength-Selectable, Electrically Driven Single-Photon Sources Operating at Room Temperature

Istvan Robel
20190236ER

Project Description

Despite its clear potential to revolutionize secure communications, the implementation of quantum cryptography is stymied by the lack of practical technologies for generating single-photons. To address this, we will develop wavelength-selectable, electrically driven, room-temperature single photon sources that exploit the unique atomic-like yet size-tunable character of electronic states in colloidal semiconductor nanocrystals. This project will leverage our recent advances in demonstrating structure-based control over recombination processes in nanomaterials in the context of electroluminescent devices. Specifically, we will develop single-nanocrystal light-emitting diodes, and use them to demonstrate a new type of room-temperature single-photon source with wavelength-selectable emission as dictated by a particular application. Successful combination of our nanomaterials and device advances, resulting in the first practical single-photon sources, will have a game-changing impact in the field of quantum information by making them as common as blue or white light-emitting diodes (LEDs), ushering in a new era of rigorous cybersecurity and ubiquitous quantum computation.

Technical Outcomes

The project team successfully accomplished the main goal of the project by demonstrating single-photon sources based on quantum dot emitters in electrically pumped prototype devices operating at room temperature. On-demand single-photon emission was accomplished by employing a pulsed electrical source. Very high electrical pumping rates have been demonstrated that, if desired, allow for the simultaneous emission of photons from two distinct quantum states – with corresponding photon energies – from an individual quantum dot.

Thermally Expandable Microspheres for Plastic-bonded Explosive (PBX) Properties Control

Amanda Duque
20190342ER

Project Description

This project aims to develop a high explosive system with shock sensitivity that may be controlled "on-demand". We will incorporate a small fraction (<1 wt%) of thermally expandable microspheres (TEMs) during the manufacturing process of the plastic-bonded explosive (PBX). The remainder of the explosive fabrication process would follow normally (i.e. pressing, casting, machining, etc), and the resulting PBX material would be in the "lower state" of shock sensitivity. That is, it would be less sensitive to insult, in particular an incoming shock wave. After exposure to a thermal stimulus (at a minimum temperature, which may be tuned by the properties of the TEM that is incorporated), either from the environment or electromagnetic energy, the TEMs would expand and decrease the local density. This creates an increase in the size and number of voids in the material, which will ultimately result in an increase in shock sensitivity. Thus, the material remains in a safer configuration until after exposure to the thermal stimulus, resulting in true "on-demand" control of explosives sensitivity.

Technical Outcomes

The project was successful in demonstrating an increase in shock sensitivity for at least one high explosive formulation containing thermally-expandable microspheres, after thermal expansion. Mesoscale reactive modeling was used to simulate the shock response of a single microsphere embedded in an explosive matrix, both before and after expansion. The results revealed an unexpected mechanism and highlighted the importance of synergistic effects of all defects at the mesoscale for predicting the effect on continuum behavior.

Publications

Journal Articles

*Higginbotham Duque, A. L., B. M. Patterson, L. A. Kuettner, S. R. Robillard, J. T. Mang and W. Lee Perry. Novel PBX formulations containing thermally-expandable microspheres for on-demand control of explosive behavior. Submitted to *AIP Conference Proceedings*. (LA-UR-19-26869 DOI: 10.1063/12.0000787)

S. Mehana, M. Z., Q. Kang, H. S. Viswanathan and H. Nasrabadi. Molecular modeling of subsurface phenomena related to petroleum engineering. Submitted to *Earth Science Reviews*. (LA-UR-20-20902)

S. Mehana, M. Z. and M. Fahes. Molecular Simulation Study of Low salinity Waterflooding Mechanisms. Submitted to *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. (LA-UR-20-20808)

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

Rai, N. K., W. L. Perry and A. L. Duque. Mesoscale Study of a Novel Method to Control Explosive Shock Sensitivity and Implications for Continuum Models. Submitted to *Journal of Applied Physics*. (LA-UR-21-31126)

*Santos, J. E., M. Mehana, H. Wu, M. Prodanovic, Q. Kang, N. Lubbers, H. Viswanathan and M. J. Pyrcz. Modeling Nanoconfinement Effects Using Active Learning. 2020. *The Journal of Physical Chemistry C*. **124** (40): 22200-22211. (LA-UR-20-22427 DOI: 10.1021/acs.jpcc.0c07427)

Reports

Rai, N. K., W. L. Perry and A. L. Duque. Mesoscale Simulation of a Novel Method to Control Explosive Shock Sensitivity and Implications for Continuum Models. Unpublished report. (LA-UR-21-30863)

Presentation Slides

Duque, A. L., B. M. Patterson, L. A. Kuettner, S. R. Robillard, J. T. Mang and W. L. Perry. Novel PBX formulations containing thermally-expandable microspheres for on-demand control of explosive behavior. Presented at *21st Biennial*

APS Topical Group on Shock Compression, Portland, Oregon, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25321)

Patterson, B. M., K. C. Henderson, N. L. Cordes, L. A. Kuettner, T. A. Shear, P. M. J. Welch, C. F. Welch, M. J. Herman, J. S. Carpenter, C. J. Montgomery, A. Ionita, N. Chawla, J. J. Williams, K. Fezzaa, T. Sun and X. Xiao. Probing Material Morphology and Deformation as a Response to In situ Loading using X-ray Tomography. Presented at *Microscopy and Microanalysis 2019*, Portland, Oregon, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27238)

Emergent Bogoliubov Fermi Surface in Unconventional Superconductors

Roman Movshovich
20190360ER

Project Description

This research will develop a new tool for superconductivity research, opening a new window into the structure of the superconducting order parameter. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion, iron-based, and high temperature cuprate superconductors.

Technical Outcomes

The team investigated thermal conductivity of heavy fermion unconventional superconductor Cerium-Cobalt-Indium 5 (CeCoIn5). Field rotation in the b-c plane revealed a rich structure in thermal conductivity (resonances and steps, dispersing with magnetic field) as a function of H rotation angle within the b-c plane. Such dispersion is expected of the Bololiubov Fermi Surfaces (BFS), observation of which with thermal conductivity is the goal of this project.

Publications

Journal Articles

Huang, Z., C. S. Ting, J. Zhu and S. Lin. Gapless Higgs Mode in the Fulde-Ferrell-Larkin-Ovchinnikov State of a Superconductor. Submitted to *Physical Review Letters*. (LA-UR-21-24876)

Kumar, U. and S. Lin. Inducing and controlling superconductivity in Hubbard honeycomb model using an electromagnetic drive. Submitted to *Physical Review B*. (LA-UR-20-30127)

Lin, S., D. Y. Kim, E. D. Bauer, F. Ronning, J. D. Thompson and R. Movshovich. Interplay of the spin density wave and a possible Fulde-Ferrell-Larkin-Ovchinnikov state in CeCoIn5 in rotating magnetic field. Submitted to *Physical Review Letters*. (LA-UR-20-23614)

*G. C. *. S. L. Zhijie, F. *., F. Zhijie and L. Shi-Zeng. Enhanced superconductivity in quasiperiodic crystals. 2021. *Physical Review Research*. **3** (2): 023195. (LA-UR-20-23148 DOI: 10.1103/PhysRevResearch.3.023195)

Organic Molecular Electrocatalysts for Hydrogen Evolution Reaction

Piotr Zelenay
20190420ER

Project Description

This project targets an entirely new class of organic molecular electrocatalysts (OMECs) for hydrogen evolution reaction (HER), an electrochemical process of fundamental importance to the future large-scale hydrogen production and processing, powered by renewable energy. The primary objectives of this work are to understand the underlying HER mechanism at metal-free OMECs, identify the structure-activity relationship for heterocyclic molecules, and enable rational design of future HER catalysts. The proposed research originates from the Laboratory's discovery of the world's first highly active OMEC for hydrogen evolution reaction that, in addition to high activity, exhibits excellent durability in an acidic polymer. In this project, the OMEC performance will be enhanced through a combination of experiments and computational modeling-guided catalyst discovery. This research is expected to conclude in a radical departure from HER electrocatalysis based on metals, either precious or non-precious. It will offer an alternative and cost-effective path to catalyzing hydrogen evolution reaction, which is essential for hydrogen production and purification. This research stands a unique chance of making a significant impact in the fields of electrocatalysis, chemistry, materials science and energy technology, in agreement with Department of Energy goals in energy conversion, including development of materials for clean-energy applications.

Technical Outcomes

This work opened new paths, concepts, and tools, from the use of metal-free catalysts, to design of catalysts using machine learning and identifying paths for further improvement of their performance using density functional theory (DFT) calculations. We have showed good agreement between these design tools and experimental results, which allows us to implement this work scheme to other challenging fields, save on design and synthesis costs, and increase the pace of projects.

Publications

Journal Articles

*Yin, X., L. Lin, U. Martinez and P. Zelenay. 2,2#-Dipyridylamine as Heterogeneous Organic Molecular Electrocatalyst for Two-Electron Oxygen Reduction Reaction in Acid Media. 2019. *ACS Applied Energy Materials*. **2** (10): 7272-7278. (LA-UR-18-27879 DOI: 10.1021/acsaem.9b01227)

Reports

Zelenay, P. Organic Molecular Electrocatalysts for Hydrogen Evolution Reaction. Unpublished report. (LA-UR-21-29641)

Presentation Slides

Yin, X. Advancing Electrocatalysts for Energy and Environmental Applications. . (LA-UR-20-20432)

Yin, X., H. Gao, E. F. Holby and P. Zelenay. Structure-Activity Data Mining for Hydrogen Evolution Reaction at Organic Molecular Electrocatalysts. Presented at *235th ECS Meeting*, Dallas, Texas, United States, 2019-05-26 - 2019-05-30. (LA-UR-19-24898)

Posters

Yin, X. Organic Molecular Electrocatalysts for Energy-Water Nexus. Presented at *2019 AIChE Annual Meeting*, Orlando, Florida, United States, 2019-11-10 - 2019-11-15. (LA-UR-19-32632)

Magnetization Fluctuation Spectroscopy as a Dynamic Probe of Emergent Magnetic Phases

Scott Crooker
20190430ER

Project Description

Magnetic materials form the basis for a huge number of essential technological applications -- for example, magnetic information storage (disk drives), certain information processing schemes (magnetic random-access memory), and sensors. New magnetic materials with exotic and potentially useful new properties are continually being developed round the world. Understanding the physics that underpins the behavior of new magnetic materials is essential if a new material is ever to be adopted as a new technology. Traditionally, this physics is revealed using conventional 'perturbative measurements', wherein the material is excited, driven, or otherwise perturbed away from equilibrium, and its response back to equilibrium is measured. Our project will establish a new and entirely alternative means of revealing the physics of magnetization dynamics -- not based on perturbation, but rather on detecting the intrinsic and ubiquitous fluctuations that naturally exist in every magnetic material. This "magnetization noise" necessarily encodes the same information (as guaranteed by the famous Fluctuation-Dissipation Theorem), and can be used to reveal the underlying magnetization dynamics without ever perturbing the system away from equilibrium, which can be particularly important near magnetic phase transitions.

Technical Outcomes

The project successfully demonstrated that 'magnetization noise' in artificial magnetic materials can indeed be detected using optical methods developed by the team. In particular, the project demonstrated that, at certain small applied magnetic fields, these materials evinced regimes wherein a dense plasma of so-called "magnetic monopoles" readily proliferated. These monopole-like particles respond to magnetic fields similarly to the way electrons respond to electric fields, opening the door to the new field of study called "magnetricity".

Publications

Journal Articles

Berman, G. P. and A. I. Nesterov. Hidden symmetries, spin and charge of artificial magnetic monopoles. Submitted to *It will be submitted to the journal: Quantum Studies: Mathematics and Foundations*. (LA-UR-21-23554)

Bian, M., A. Kamenskii, S. A. Crooker and H. Zeng. Atomically-thin Cr2Te3 Ferromagnet - a 2D Half-Metal. Submitted to *Nano Letters*. (LA-UR-20-26568)

*Chernyak, V. Y., F. Li, C. Sun and N. A. Sinitsyn. Integrable multistate Landau–Zener models with parallel energy levels. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (29): 295201. (LA-UR-20-20621 DOI: 10.1088/1751-8121/ab9464)

*Cristiano, N. Topological order of the Rys F-model and its breakdown in realistic square spin ice: Topological sectors of Faraday loops. 2020. *EPL (Europhysics Letters)*. **132** (4): 47005. (LA-UR-20-20959 DOI: 10.1209/0295-5075/132/47005)

*Goryca, M., X. Zhang, J. Li, A. L. Balk, J. D. Watts, C. Leighton, C. Nisoli, P. Schiffer and S. A. Crooker. Field-Induced Magnetic Monopole Plasma in Artificial Spin Ice. 2021. *Physical Review X*. **11** (1): 011042. (LA-UR-20-24139 DOI: 10.1103/PhysRevX.11.011042)

Nisoli, C. The color of magnetic monopole noise. 2021. *EPL (Europhysics Letters)*. (LA-UR-20-24778 DOI: 10.1209/0295-5075/ac2654)

Sinitsyn, N., A. Fisher, I. Kleinjoharnn and F. B. Anders. Cross-correlation spectra in interacting quantum dot systems. Submitted to *Physical Review B*. (LA-UR-21-28148)

Yan, B., V. Y. Chernyak, W. H. Zurek and N. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. Submitted to *Physical Review Letters*. (LA-UR-20-26742)

Yan, B. and N. Sinitsyn. Recovery of damaged information and the out-of-time-ordered correlators. Submitted to *Physical Review Letters*. (LA-UR-20-22064)

Presentation Slides

Crooker, S. A. Listening to spin and magnetization noise. . (LA-UR-20-29529)

Crooker, S. A. Electrons, Holes, & Excitons in Monolayer Semiconductors (insights from spectroscopy in *really* large magnetic fields). Presented at *OECS*, virtual (Dortmund), Germany, 2021-08-30 - 2021-08-30. (LA-UR-21-29035)

Sinitsyn, N. Correlators of electronic spins. Presented at *MCR Workshop*, Los Alamos, New Mexico, United States, 2021-04-30 - 2021-04-30. (LA-UR-21-24199)

Mixed Conductors for Enhanced Fuel Cell Performance

Yu Seung Kim
20190440ER

Project Description

This project addresses energy security issues by improving the performance and reducing the cost of zero-emission energy conversion devices. The goal of the research is to develop improved catalyst supports for fuel cell applications. By enabling the support to conduct electrons and protons at the same time, we will enable higher performance with lower cost, leading to accelerated deployment of fuel cell technology for transportation and defense applications.

Technical Outcomes

From this project, we developed functionalized mixed conductors (FMCs) for polymer electrolyte membrane fuel cells (PEMFCs). The FMCs eliminate the need for a triple phase boundary and enable the design of ionomer-free electrodes with simplified interfaces. We demonstrated that PEMFCs using the ionomer-free electrodes based on FMCs showed improved oxygen transport and ORR kinetics, leading to dramatic increases in fuel cell performance compared to ionomer-free electrode based on commercial catalysts.

Publications

Journal Articles

Li, D., Y. Pan, X. Wang, C. Wang, Y. S. Kim and J. S. Spendelow. Effect of the Catalyst Metal Content on PEMFC Durability. Submitted to *ECS Transactions*. (LA-UR-19-27318)

*Maurya, S., A. S. Lee, D. Li, E. J. Park, D. P. Leonard, S. Noh, C. Bae and Y. S. Kim. On the origin of permanent performance loss of anion exchange membrane fuel cells: Electrochemical oxidation of phenyl group. 2019. *Journal of Power Sources*. **436**: 226866. (LA-UR-19-23575 DOI: 10.1016/j.jpowsour.2019.226866)

Three-dimension (3-D) Printed Hierarchically Porous Heat Pipe Wicks

Matthew Lee
20190463ER

Project Description

This project aims to develop a new class of heat transfer materials with enhanced properties and performance metrics suitable for a wide range of engineering applications. Using three-dimensional (3-D) printing techniques recently pioneered by members of our team, the goal of this project is to generate novel metallic wicking materials for heat pipes with optimized structural geometries and a vastly broadened design space.

Heat pipes are key components in many technologies pertinent to the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) and other government agencies, including waste heat recovery, nuclear energy, space applications and high performance computing. Therefore, this research directly addresses current national security challenges in energy security, aerospace and defense applications. In addition, this research can potentially lead to the large-scale manufacturing of more compact and efficient heat pipe designs with increased capacity to transport thermal energy, thereby broadening the span of their end-use applications and advancing key technologies already used through the DOE complex and beyond. Through our research we aim to identify key parameters governing heat pipe performance, optimize these through the use of 3-D printing, and pave the way toward new heat pipe designs and applications that were not possible until now.

Technical Outcomes

Until now, wick materials have been formed simply by sintering metal particles together in a random arrangement, or often rolling metal screens up in a tube-like configuration. The results of this project demonstrate that far more sophisticated wick structures are possible via the combination of complex fluid self-assembly and light-based additive manufacturing. These results certainly warrant further investigation and integration into small scale devices in future years. A provisional patent has been filed.

Superdetonation Shaped Charges

Shawn Mcgrane
20200124ER

Project Description

Shaped charges are widely used by the military to defeat armor, breach barriers, and destroy unexploded ordnance. Shaped charges are also widespread in oil and gas well perforation. Due to these prominent applications, there has been continuous research into new methods of improving shaped charge capabilities. We recently patented an idea to use the phenomenon of superdetonation to increase explosive performance for shaped charge applications. While the detonation velocity of nitromethane is 6.2 kilometers per second (km/s), the superdetonation velocities can be up to 13 km/s. This is substantially higher than currently available high performance explosives, that have detonation velocities up to ~9 km/s. We will build, test, and optimize the first explosively driven shaped charges that use superdetonation to nearly double the performance of currently available explosives.

Technical Outcomes

The team completed three design iterations, builds, and dynamic testing series in the development of superdetonation shaped charges. During the design iterations, significant advances were made in nitromethane modeling development and waveshaper design that were not intended aspects of the original project.

Publications

Reports

Mcgrane, S. D. Superdetonation shaped charges. Unpublished report. (LA-UR-22-20432)

Additive Manufacturing of 3-Dimensional and Graded Density Explosive Structures

Dana Dattelbaum
20200632ER

Project Description

The development of Additive Manufacturing technologies for the production of High Explosive (HE) charges has allowed for the introduction of new functionalities into previously brute force materials. The discovery of mechanisms to introduce directional sensitivity, detonation steering and control and structurally mediated initiation regions promise the development of safer and more useful explosive charges. With previous work having discovered methods of introducing such functionality, more exploration is necessary to fully exploit the extensive possibilities enabled by this new manufacturing technique.

Technical Outcomes

This project demonstrated the manufacturability and reactive burn characteristics of a new Additively Manufactured High Explosive (AM-HE) formulation, AMX 7301. The explosive was found to be printable into booster-like shapes. The shock sensitivity was found to be less sensitive than the High Melting eXplosive (HMX)-based formulation PBX (Plastic-bonded Explosive) 9501, owing to its lower HMX content, and more ductile binder system. The data will be used to parameterize reactive burn models to be used in predicting its behavior in modular booster components

Publications

Reports

Dattelbaum, D. M., A. H. Mueller, L. L. Gibson and A. M. Schmalzer. Additive Manufacturing of 3-Dimensional and Graded Density Explosive Structures. Unpublished report. (LA-UR-21-24814)

Presentation Slides

Brown, C. B. Microstructure Characterization of Additive-Manufactured PBX. . (LA-UR-20-22869)

Nguyen, T. D., B. C. Tappan, A. M. Schmalzer, D. E. Chavez and A. H. Mueller. A New Route to a Highly Energetic Binder for Additive Manufacturing. Presented at *6th Cross-JOWOG Working Group Meeting on Applications, Design, and Certification of Additive Manufacturing for the Stockpile*, Kansas City, Missouri, United States, 2022-02-28 - 2022-02-28. (LA-CP-22-20105)

Engineering Nanoionic Memristive Functionality in 3-Dimensional (3D) Oxide Heterostructures

Dmitry Yarotski
20210733ER

Project Description

Memristors (memory+resistor), two-terminal electronic elements that remember their most recent resistance state, hold the key to novel computing architectures and non-volatile memory devices. In this work, we will (i) couple a unique-to-Los Alamos National Laboratory suite of atomistic Accelerated Molecular Dynamics (AMD) methods to mesoscale density functional theory (DFT)-informed Tight-Binding Multiscale Material Modeling (TBM3) framework to simulate ionic motion along the interfaces and its effect on electronic charge transport under electric field in exemplary 3-Dimensional nanocomposites of Titanium dioxide (TiO_2)/Strontium titanate ($SrTiO_3$); (ii) synthesize most promising TiO_2/$SrTiO_3$ 3D structures; and (iii) apply high-resolution probes to validate theoretical predictions and further refine our multiscale modeling toolset. The best performing memristors will be integrated into the small networks following (iv) predictions from the architecture modeling in order to set the limits on the acceptable variation of single element properties for reliable operation of neuromorphic (nm) grids. Such a "nm-to-architecture" approach has never been applied before and will result in development of the scientific principles that underpin the memristive response of oxide nanocomposites and enable a rational design of "memory" materials with optimal device and grid performance.

Technical Outcomes

The team demonstrated feasibility of multi-scale modeling of memristive response of heterostructures with subsequent validation using advanced synthetic and photoemission techniques. These results serve as a basis for further development of integrated co-design framework for discovering the scientific principles that underpin the memristive response and enable a rational design of "memory" materials with optimal device and grid performance. This framework will provide Los Alamos with a capability for accelerated materials discovery well beyond memristor applications.

Publications

Journal Articles

Rutherford, B. X. Implementing ceramic materials into neuromorphic memory devices through oxide-based memristors. Submitted to *American Ceramic Society Bulletin*. (LA-UR-21-25583)

Yun, C., M. Webb, w. li, R. Wu, M. Xiao, M. Hellenbrand, A. Kursumovic, H. Dou, X. Gao, S. Dhole, D. Zhang, A. Chen, J. Shi, K. Zhang, H. Wang, Q. Jia and J. L. MacManus-Driscoll. High performance, electroforming-free, thin film memristors using ionic $Na_{0.5}Bi_{0.5}TiO_3$. Submitted to *Journal of Materials Chemistry C*. (LA-UR-21-22721)

Reports

Chen, A. In Operando Study of Resistive-switching Devices at Nanoscale. Unpublished report. (LA-UR-21-24776)

Embedded Sensing and Monitoring Techniques for Small Modular Reactors

Timothy Ulrich
20210802ER

Project Description

As new nuclear reactor technologies emerge in the fight for more efficient electricity production worldwide, innovative techniques for assessing reactor behavior, especially in significantly smaller reactor designs than are currently seen at commercial Light Water Reactor facilities become increasingly important. The goal of this project is to develop innovative instrumentation techniques for assessing parameters needed for safe small modular reactor operation and safeguarding of nuclear material. New advanced reactor designs are often sealed on deployment and not accessible again until disposal. This work aims to use embedded acoustic and fiber optic sensors to monitor the integrity of reactor fuel and body structure to allow for constant monitoring without requiring access to the reactor, with the possibility of continued monitoring after reactor shutdown. These techniques have been demonstrated in other applications, and this project will test the techniques to ensure their performance and capabilities in the unique small modular reactor environment.
The small (in size not capability), powerful techniques proposed in this research could greatly aid reactor vendors in designing equipment for core measurements throughout the lifetime and following materials accountability after shutdown of a small modular reactor.

Technical Outcomes

This project successfully demonstrated the use of resonant ultrasound spectroscopy and nonlinear resonant ultrasound spectroscopy for monitoring mechanical properties and integrity using ambient noise excitation. Additionally, the necessary vibrational signals were demonstrated to be measurable using fiber Bragg gratings, an optical sensing technology that can be readily employed as an embedded sensor array in extreme conditions. Finally, optically sensed luminescence was demonstrated as a feasible means for measuring radiation dose in in situ reactor conditions.

Publications

Presentation Slides

I. Ulrich, T. J., M. Remillieux, L. B. Beardslee and P. Le Bas. Physical Acoustics Characterization For Inspection and Evaluation. . (LA-UR-21-24510)

Overcoming the Barriers for Growing Device Quality Ultrawide Bandgap Gallium Oxide Semiconductors

Mark Hoffbauer
20210951ER

Project Description

Wide bandgap (WBG) semiconductors are rapidly emerging as key materials that can dramatically increase energy efficiency, improve device performance, and lower costs across a wide range of energy applications. Next generation ultrawide-bandgap (UWBG) semiconductor materials including aluminum gallium nitride/aluminum nitride (AlGaN/AlN), Gallium Oxide (Ga_2O_3), and diamond have the potential for far superior performance. Thus, there are strong motivations and emerging opportunities for further developing Ga_2O_3 semiconductors, but progress in developing Ga_2O_3-based semiconductor devices has been severely constrained by the availability of epitaxial Ga_2O_3 crystalline thin films due to limitations of conventional growth processes. An exclusive thin film growth capability developed at LANL will be utilized to remove these constraints to make Ga_2O_3 single crystal films at high growth rates and at lower growth temperatures. Breakthrough results are expected that will open new opportunities and applications for high performance UWBG oxide semiconductors. These advancements in WBG/UWBG semiconductor materials will revolutionize the next generation of power electronics and clean energy innovations across national defense and energy security applications while providing United States manufacturers a competitive edge in growing markets for a new and powerful semiconductor material.

Technical Outcomes

The project goals were met by demonstrating that highly crystalline Gallium oxide semiconducting films can be grown at rates up to 4 microns/hour and at temperatures as low as 500 Celsius. It was shown that the Gallium oxide films can be Germanium doped at high levels of a few atomic percent for use in devices offering improved high voltage switching performance. Improvements in advanced ultra-wide bandgap semiconductors have broad applications across energy and national security arenas.

Adaptive Framework for Enabling Real-time Feedback During Three-dimensional Mesoscale Microstructure Evolution Measurements

Reeju Pokharel
20190571ECR

Project Description

This project will develop a data analysis framework that will revolutionize experiments and data analysis at current and future light sources. This project will combine state-of-the-art measurement techniques, machine learning based data analysis tools, measurement informed mechanics simulations, and adaptive model independent optimization methods to enable real-time feedback during microstructure evolution studies at light sources. The ability to provide real-time feedback during a beam line experiment will be crucial for guiding experiments that can provide information that will be crucial for influencing predictive model development. The framework will maximize the productivity and impact of a beam time and will have broad programmatic and mission impacts. Results will also be of significant interest to the light source user community and numerous collaborations will emerge as an outcome.

Publications

Journal Articles

Pandey, A., J. G. Gigax and R. Pokharel. Machine learning force-field to develop and optimize multi-components alloys. Submitted to *Computational Materials Science*. (LA-UR-22-20252)

Pandey, A. and R. Pokharel. Spatially resolved 3D microstructure evolution using long short-term memory. Submitted to *International Journal of Plasticity*. (LA-UR-20-23111)

Pandey, A. and R. Pokharel. Machine learning based surrogate modeling approach for mapping crystal deformation in three dimensions. Submitted to *Scripta Materialia*. (LA-UR-20-25246)

Pokharel, R., A. Pandey and A. Scheinker. Physics-informed data-driven surrogate modeling for full-field 3D microstructure and micro-mechanical field evolution of polycrystalline materials. Submitted to *JOM*. (LA-UR-21-25674)

Presentation Slides

R. Castillo, J. A. HEDM Reconstruction Problem. Presented at *Weekly meeting*, Los Alamos, New Mexico, United States, 2019-06-18 - 2019-06-18. (LA-UR-19-25507)

R. Castillo, J. A. Fourier Dictionary Approach for HEDM reconstruction. Presented at *weekly meeting with advisor*, Los Alamos, New Mexico, United States, 2019-07-23 - 2019-07-24. (LA-UR-19-27031)

Pandey, A. Physics-informed data-driven surrogate modeling for advancing experiments and the study of novel materials. . (LA-UR-21-27990)

Pandey, A. and R. Pokharel. Real-time analysis of diffraction data for enabling in-situ measurements. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-22416)

Pandey, A. and R. Pokharel. Physics-informed Data-driven Surrogate Modeling for Advancing Experiments and the Study of Novel Materials. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-27 - 2022-03-03. (LA-UR-22-21816)

Pokharel, R. Data analysis framework for enabling real-time feedback during microstructure evolution. Presented at *IMS Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23306)

Pokharel, R. 3D microstructure characterization using high-energy X-rays. Presented at *3D Summer School*, Pittsburgh, Pennsylvania, United States, 2019-08-19 - 2019-08-19. (LA-UR-19-28333)

Pokharel, R. Physics-informed Data-driven Machine Learning Approach for Mesoscale Materials Science. Presented at *TMS*, Orlando, Florida, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22695)

Pokharel, R. Machine learning for real-time 3D characterization of mesoscale materials. Presented at *Engineering, Structural, and Geological Materials from Processing to Performance Workshop*, Ithaca, New York, United States, 2021-07-13 - 2021-07-13. (LA-UR-21-26437)

Plutonium Defect Characterization through Mechanical Deformation

Taylor Jacobs
20200557ECR

Project Description

Defects in a material heavily influence properties, such as strength, ductility, and toughness that are vital to engineering applications. Radiation damage occurs naturally in plutonium through radioactive decay and introduces defects over time. The characterization of defect structures in plutonium alloys during such aging is vital to the Department of Energy/National Nuclear Security Administration/Los Alamos National Laboratory strategic goal to provide a safe, secure, and effective nuclear stockpile. To this end many experimental and modeling efforts have been made to understand defect evolution during plutonium aging. Unfortunately, plutonium aging is a complex problem and a complete understanding of defect-property relationships have remained elusive. This project seeks to introduce stress relaxation and internal friction experiments to plutonium metallurgy. These mechanical testing experiments are robust, well-developed defect characterization techniques that complement the nation's existing efforts to understand aging phenomena. The team expects to see detectable changes in defect interactions in plutonium samples with different ages and processing conditions. The experimental matrix is designed to separate effects from processing and aging by working with well-characterized material from previous studies and performing a parallel set of experiments on aluminum and copper alloys that are designed to have specific defects that are relevant to plutonium.

Publications

Presentation Slides

Jacobs, T. R. A Plutonium Mechanical Strength Model that Parallels Stress Relaxation Experiments. Presented at *Colorado School of Mines Invited Student Seminar Series*, Golden, Colorado, United States, 2022-03-17 - 2022-03-17. (LA-UR-22-22097)

Jacobs, T. R., M. J. Gibbs, C. A. Yablinsky, F. J. Freibert, S. C. Hernandez, J. N. Mitchell, T. A. Saleh, G. A. Kral, E. M. Solis, S. D. Imhoff, J. S. Bridgewater and D. F. Teter. Defects and Mechanical Behavior of Plutonium. . (LA-UR-20-22799)

Synthesis of Aluminum Clusters as Next Generation Explosives

Christopher Snyder
20200560ECR

Project Description

The development of new explosives with more energy than current conventional materials is important in national security. In the 156 years since the development of TNT (Trinitrotoluene), the most powerful explosive to date, CL-20 (hexanitrohexaazaisowurtzitane), is marginally better, with a detonation velocity that is only 33% higher than TNT. These materials, and most conventional explosives, are based on the elements carbon, hydrogen, nitrogen, and oxygen (CHNO). Despite the development of thousands of CHNO explosives since the discovery of TNT, obtaining an explosive with drastically better explosive properties has not been achieved. Therefore, a new approach needs to be developed to synthesize new explosives that incorporate materials that can provide better explosive performance. Aluminum-based materials have the potential to be superior to conventional explosives because aluminum has one of the highest energy densities of any material. The ultimate goal of this project is to develop aluminum clusters capped by oxygen-rich ligands as next generation explosive materials. Upon initiation, the aluminum core will react with the oxygen-rich ligands, which is predicted to release more energy than conventional explosives alone. These materials would be useful in detonators and booster applications, where there is a current need for more powerful explosive materials.

The Role of Defects in Mechanical Instabilities of Additively Manufactured Lattice Materials

Rachel Collino
20200588ECR

Project Description

3-Dimensional (3D) printing has enabled the realization of geometries that were otherwise difficult or impossible to produce via traditional manufacturing techniques, including lattice materials (periodic truss structures). These structures are promising for creating lightweight materials with exceptional strength or energy absorption characteristics, but additively-manufactured lattice materials often fall short of their predicted performance. This performance gap, lack of reproducibility in mechanical behavior, and absence of a framework for part qualification all hinder the widespread adoption of lattice materials within the Department of Energy (DOE) complex. This work will use high-resolution printing techniques to create structures with intentional defect geometries, in tandem with X-Ray Computed Tomography (XCT) to observe complex structural deformations and damage evolution in 3D, to enable systematic studies of defect shape and location on failure initiation in these materials. The results will inform both simple models for screening designs (what combinations of lattice arrangement, material, and printing defects are unacceptable for a given performance criterion) as well as efforts in in-situ diagnostic development and science-based qualification.

Publications

Journal Articles

Dong, C. Q., R. R. Collino, S. P. Donegan, J. D. Miller and M. R. Begley. Effective properties for millimeter-scale struts and strut intersections (nodes) fabricated via EBM. Submitted to *TBD*. (LA-UR-21-27634)

Presentation Slides

Collino, R. R., K. J. Cluff, E. A. Sandoval, R. A. (. Mikofsky, S. L. Young, L. A. Kuettner, M. N. Lee, C. J. Montgomery and B. M. Patterson. LDRD Early Career Project Update: The role of defects in mechanical instabilities of additively-manufactured lattice materials. . (LA-UR-21-27567)

Kick-Starting the Hydrogen Economy with Transition Metal Nitrides

John Watt
20210604ECR

Project Description

Low-cost, high activity, stable electrocatalysts for water splitting are essential for the economical production of hydrogen (H2) as a high density, carbon neutral fuel. The bottleneck to achieving industrially relevant efficiency for the two component processes (hydrogen and oxygen production) is the sluggish oxygen evolution reaction (OER) at the anode. Recent studies have reported transition metal nitride (TMN) nanoparticles (NPs) with remarkably improved activity for the OER over current industry standards. However, these materials require harsh reaction conditions to form, which make it difficult to control NP composition and morphology. This lack of tight synthetic control has precluded any mechanistic understanding of their catalytic performance. A new synthetic pathway to TMN NPs must be developed, along with methods for real-time observation of structural changes during catalysis, to enable systematic analysis of fundamental structure-function relationships. This will lead to earth-abundant OER catalysts that can be actively designed to have better performance than noble metals.

Strain-driven Demonstration of Chiral Superconductivity

Sean Thomas
20210607ECR

Project Description

Quantum information science is a key research area for the nation's energy and security interests. A promising route to quantum computation is to build a quantum bit using a so-called Majorana mode. A class of superconductors, called chiral superconductors, are predicted to host these Majorana modes, but unambiguous evidence of chiral superconductivity remains to be demonstrated. The goal of this project is to provide definitive proof of the chiral superconducting state through development of a new capability. This will be accomplished by combining heat capacity and uniaxial strain with a specialized optical technique.

Publications

Posters

M. Girod, C. P., S. M. Thomas, P. Rosa, F. Ronning, E. D. Bauer, J. D. Thompson, A. Huxley and C. Stevens. Mapping superconductivity with uniaxial stress in UTe2. Presented at *2022 Aspen Winter Conference, New Directions in Strong Correlation Physics: From Strange Metals to Topological Superconductivity*, Aspen, Colorado, United States, 2022-01-24 - 2022-01-28. (LA-UR-22-20243)

Strong and Ductile: Towards a New Class of High Entropy Alloys with Outstanding and Optimized Properties

Osman El Atwani
20210626ECR

Project Description

This project possesses interconnected experimental and modeling elements to generate a detailed understanding of chemistry and composition on the ductility of refractory four elemental alloys to optimize the performance of these alloys under extreme environments. The possible combination of elements to synthesize a four elemental alloy is virtually infinite. However, the elements are chosen to minimize radioactivity for nuclear applications. The alloys to be studied are Tungsten-Tantalum-Chromium-Vanadium (W-Ta-Cr-V) and Tungsten-Tantalum-Chromium-Iron (W Ta-Cr-Fe). These alloys will be formed in different compositions and the ductility of these alloys will be investigated. For compositions that demonstrate high ductility, other tests (such as irradiation and thermal stability) will be performed. Effect of composition on the performance of these materials will be then understood and a design of a high performance four elemental alloy will be possible.

Publications

Journal Articles

El Atwani, O., H. Kim, C. R. Harvey, M. Efe and S. A. Maloy. Limitations of Thermal Stability Analysis via In-Situ TEM/Heating Experiments. 2021. *Nanomaterials*. **11** (10): 2541. (LA-UR-21-29330 DOI: 10.3390/nano11102541)

El Atwani, O., H. Kim, J. G. Gigax, C. R. Harvey, B. Aytuna, M. Efe and S. A. Maloy. Highly Stable, Ductile and Strong Nanocrystalline HT-9 Steels via Large Strain Machining. Submitted to *Materials & Design*. (LA-UR-21-28477)

Aydogan, E., O. El Atwani, B. Erdem, W. Chen, M. Li, A. Devaraj, B. Koc and S. A. Maloy. In-situ radiation response of additively manufactured modified Inconel 718 alloys. Submitted to *Additive Manufacturing*. (LA-UR-21-29969)

Bergstrom, Z. J., D. Perez and O. El Atwani. Helium bubble facetation in tungsten thin films. Submitted to *Scripta Materialia*. (LA-UR-22-20655)

Iroc, L., O. El Atwani, M. A. Tunes, Y. Kalay and E. Aydogan. Enhancement of the strength-ductility trade-off by transformation-induced nanolamellar structures and nanotwinning in oxygen-doped TiZrHfNbTa refractory high-entropy alloys. Submitted to *Advanced Materials*. (LA-UR-22-21273)

Computational Modeling for the Development of Chiral Quantum Systems

Amanda Neukirch
20210672ECR

Project Description

The term chirality is derived from the Greek word for hand and applies to any object that differs from its mirror image. All known living things are chiral. This project will study the chiroptical properties of organic ligand capped semiconductor and metallic quantum dots as they possess unique yet modular structural and optical properties not present in bulk materials. These systems are promising candidates for a broad range of applications such as drug screening, security surveillance, remote sensing, and quantum optics. Two things are needed for a direct circularly polarized light (CPL) photodetector to perform well. The first is that the absorber needs to combine handedness sensitive optical absorption (typically obtained via chiral organic ligands). The second is efficient charge transport (often best achieved with semiconductor or metallic systems). This proposal will allow for the achievement of the best of both worlds and determine structure property relationships that will allow for the controlled development of quantum chiral systems.

Publications

Journal Articles

. G. D. *. J. K. L. *. F. D. *. S. A. *. L. S. G. *. L. F. *. N. W. *. B. J. *. Z. L. *. C. J. J. *. M. N. *. M. A. D. *. T. S. *. N. A. J. Lewis, S. G., S. G. Lewis, D. Ghosh, F. Liu, W. Nie, L. Zhou, J. J. Crochet, S. Tretiak, A. J. Neukirch and N. Moody. Cesium-Coated Halide Perovskites as a Photocathode Material: Modeling Insights. 2021. *The Journal of Physical Chemistry Letters*. **12 (27): 6269-6276. (LA-UR-21-24212 DOI: 10.1021/acs.jpclett.1c01412)

Mora Perez, C. A., D. Ghosh, O. Prezhdo, W. Nie, S. Tretiak and A. J. Neukirch. Point Defects in 2D Ruddlesden-Popper Perovskties Explored with ab initio Calculations. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-22-21646)

Reports

Neukirch, A. J., D. Ghosh, C. A. Mora Perez, O. Prezhdo, W. Nie and S. Tretiak. Impact of Compositional Engineering on Charge Carrier Cooling in Hybrid Halide Perovskites: Computational Insights. Unpublished report. (LA-UR-22-20401)

Presentation Slides

Forde, A. A. Excited state dynamics of photo-induced polarons in lead halide perovskite nanocrystals: Bright surface-trap states\xe2\x80\xaf\xc2\xa0. Presented at *The International Chemical Congress of Pacific Basin Societies (Pacifichem)*, Honalulu, Hawaii, United States, 2021-12-19 - 2021-12-19. (LA-UR-21-32290)

Forde, A. A. Induced Chirality in Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *Sanibel Symposium*, St. Simons Island, Georgia, United States, 2022-02-13 - 2022-02-18. (LA-UR-22-21246)

Neukirch, A. J. Nonadiabatic Dynamics Shines Light on How to Best Harness Perovskite Properties for Use in Optoelectronic Properties. Presented at *Nonequilibruim Phenomena, Nonadiabatic Dynamics and Spectroscopy*, Telluride, Colorado, United States, 2021-07-19 - 2021-07-23. (LA-UR-21-26972)

Neukirch, A. J., A. A. Forde, D. Ghosh, A. C. Evans and S. Tretiak. Chirality Transfer Induced in a Lead-Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *Pacifichem 2021*, Virtual, New Mexico, United States, 2021-12-16 - 2021-12-21. (LA-UR-21-32289)

Neukirch, A. J., A. A. Forde, D. Ghosh, D. S. Kilin, A. C. Evans and S. Tretiak. Chirality Transfer Induced in a Lead-Halide Perovskite Cluster Through Surface Chemistry Modification. Presented at *APS March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22483)

Posters

Forde, A. A. Improving Near-Infrared Fluorescence Quantum Yield of meso-Aryldipyrrin Indium(III) Complexes via Annulation Bridging: A Non-Adiabatic Excited-State Dynamics Study. Presented at *Sanibel Symposium*, St. Simons Island, Georgia, United States, 2022-02-13 - 2022-02-18. (LA-UR-22-21139)

Forde, A. A., A. C. Evans, S. Tretiak and A. J. Neukirch. Towards Implementation of Modified-Redfield Theory into ab Initio Excited-State Dynamics. Presented at *Sanibel Sympsium*,

St. Simons Island, Georgia, United States, 2022-02-13 -
2022-02-18. (LA-UR-22-21138)

Electronic Transport in Atomically Thin Materials at Far from Mechanical Equilibrium Conditions

Michael Pettes
20190516ECR

Project Description

Transition metal dichalcogenides (TMDs) are particularly sensitive to mechanical strain as they are capable of experiencing high strains without nucleating defects to release excess energy. As both the effective mass and optical phonon energies in these materials decrease with strain, and since the electron lifetime is inversely proportional to the phonon energy and occupation, an increase of electron mobility is hypothesized to occur with tensile elastic strain. This is significant as the drift velocity directly determines the switching speed in ultra-fast transistors as well as excitonic recombination dynamics in nano photonic devices. This research will address the fundamental question of how the variable of strain influences electronic performance in 2-dimensional materials, so that it can be fully accounted for in the design of next-generation nano electronic devices. Upon completion of this project, the PI will have established a globally unique in situ TEM-based structure-property characterization capability to quantify and correlate atomic-level strain experienced by a suspended nano material with electronic transport properties, a technique currently not possible and very relevant to structure-processing-property testing of other thin films including actinide-based materials required for advanced weapons and sensor applications.

Technical Outcomes

The outcome of this project has been three-fold: (i) discovery of strain-driven quantum emission in a 2D material through new device fabrication to impart strain locally at the nanoscale, (ii) implementation of four dimensional transmission electron microscopy at Los Alamos, and (iii) synthesis of a new air stable 2D material with promising non-linear optical properties. This has resulted in the building of a complex new experimental laboratory at Los Alamos National Laboratory.

Publications

Journal Articles

*Pettes, M. T., A. Londono Calderon, D. J. Williams, B. H. Savitzsky, C. Ophus, S. Ma, H. Zhu and M. M. Schneider. Intrinsic helical twist and chirality in ultrathin tellurium nanowires. 2021. *Nanoscale*. **13** (21): 9606-9614. (LA-UR-21-21904 DOI: 10.1039/D1NR01442K)

*Pettes, M. T., A. Londono Calderon, D. J. Williams, C. Ophus, B. Savitsky and M. M. Schneider. Local Lattice Deformation of Tellurene Grain Boundaries by Four-Dimensional Electron Microscopy. 2021. *The Journal of Physical Chemistry C*. **125** (6): 3396-3405. (LA-UR-20-27603 DOI: 10.1021/acs.jpcc.1c00308)

*Pettes, M. T., A. Londono Calderon, D. J. Williams and C. Ophus. 1D to 2D Transition in Tellurium Observed by 4D Electron Microscopy. 2020. *Small*. **16** (49): 2005447. (LA-UR-20-25292 DOI: 10.1002/smll.202005447)

Pettes, M. T., A. Londono Calderon, R. Dhall, C. Ophus, Y. Wang, E. Dervishi-Whetham, H. S. Kang, C. Lee and J. Yoo. Visualizing Grain Statistics in MOCVD WSe through Four-Dimensional Scanning Transmission Electron Microscopy. 2022. *Nano Letters*. (LA-UR-21-30267 DOI: 10.1021/acs.nanolett.1c04315)

*Wei, W., C. K. Dass, J. R. Hendrickson, R. D. Montano, R. E. Fischer, Z. Xiaotian, T. H. Choudhury, J. M. Redwing, W. Yongqiang and M. T. Pettes. Locally defined quantum emission from epitaxial few-layer tungsten diselenide. 2019. *Applied Physics Letters*. **114** (21): 213102. (LA-UR-18-27142 DOI: 10.1063/1.5091779)

*Yazdani, S., R. Kashfi-Sadabad, M. D. Morales-Acosta, R. D. Montano, N. V. Tuoc, D. T. Huan, M. Zhou, Y. Liu, J. He and M. T. Pettes. Thermal transport in phase-stabilized lithium zirconate phosphates. 2020. *Applied Physics Letters*. **117** (1): 11903. (LA-UR-20-24103 DOI: 10.1063/5.0013716)

P. M. T. *. Z. Y. *. H. H. Zhao, H. *., H. Zhao, M. T. Pettes, Y. Zheng and H. Htoon. Site-controlled telecom-wavelength single-photon emitters in atomically-thin MoTe2. 2021. *Nature Communications*. **12** (1): 6753. (LA-UR-21-23958 DOI: 10.1038/s41467-021-27033-w)

Presentation Slides

Londono Calderon, A., C. Ophus, D. J. Williams and M. T. Pettes. Quantifying peak profile analysis of 2D Tellurium nanostructures by 4D-STEM. Presented at *2020 virtual MRS Spring/Fall meeting & exhibit*, Los Alamos, New Mexico, United States, 2020-11-27 - 2020-12-04. (LA-UR-20-29012)

Londono Calderon, A., D. J. Williams, B. H. Savitzky, C. Ophus, S. Ma, H. Zhu, M. M. Schneider and M. T. Pettes. Intrinsic Helical Twist and Chirality in Ultrathin Tellurium Nanowires. Presented at *2021 Microscopy & Microanalysis*, Pittsburgh, Pennsylvania, United States, 2021-08-01 - 2021-08-05. (LA-UR-21-21748)

Londono Calderon, A., D. J. Williams, B. H. Savitzky and M. T. Pettes. Towards Crystallographic Orientation and Strain Mapping of 1D & 2D Tellurium from 4D-STEM. Presented at *Microscopy & Microanalysis 2020 virtual meeting*, Los Alamos, New Mexico, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-25117)

Pettes, M. T. Deterministic Defect Emission from Epitaxial TMD Thin Films. Presented at *Invited Seminar at 2D Crystal Consortium-Materials Innovation Platform NSF Site Visit Year 4*, University Park, Pennsylvania, United States, 2019-05-21 - 2019-05-21. (LA-UR-19-24535)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited seminar at University of California, Merced Mechanical Engineering Department*, Merced, California, United States, 2019-09-27 - 2019-09-27. (LA-UR-19-29644)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited Seminar at North Carolina State University Mechanical Engineering Department*, Raleigh, North Carolina, United States, 2019-10-18 - 2019-10-18. (LA-UR-19-30501)

Pettes, M. T. Deterministic Quantum Emission in an Epitaxial 2D Material. . (LA-UR-19-25907)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited Seminar at Yale University Energy Sciences Institute*, New Haven, Connecticut, United States, 2019-07-30 - 2019-07-30. (LA-UR-19-27328)

Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials: WSe2 and Te. Presented at *Invited Seminar at Rice University Materials Science Department*, Houston, Texas, United States, 2020-01-16 - 2020-01-16. (LA-UR-20-20408)

Pettes, M. T. Emergent Phenomena in van der Waals Materials: Advancements in Characterization. Presented at *Invited Seminar presented to the University of Minnesota*, Minneapolis (online), Minnesota, United States, 2020-10-28 - 2020-10-28. (LA-UR-20-28618)

Pettes, M. T. Towards control over 2D material properties through ion beam modification and analysis. Presented at *CINT 2021 Annual Meeting*, Online, New Mexico, United States, 2021-09-21 - 2021-09-21. (LA-UR-21-29318)

Posters

Londono Calderon, A., D. J. Williams and M. T. Pettes. Strain mapping of grain boundary in two-dimensional tellurene by 4D-STEM. Presented at *2020 CINT Annual Meeting*, Online, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27301)

Pettes, M. T. Intrinsic and Extrinsic Control over Physical Properties in a Representative Atomically Thin Semiconductor. Presented at *2019 National Academy of Engineering EU-US Frontiers of Engineering symposium*, Stockholm, Sweden, 2019-11-18 - 2019-11-20. (LA-UR-19-31073)

Pettes, M. T., A. Londono Calderon and D. J. Williams. Crystallographic Orientation of 1D & 2D Tellurium from 4D Scanning Transmission Electron Microscopy. Presented at *13th Annual Postdoctoral Technical Showcase, Sandia National Laboratories*, Albuquerque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-32519)

Nonlinear Photonics of Topological Phase Transitions in the Graphene Family

Wilton Junior de Melo Kort-Kamp
20190574ECR

Project Description

Topology studies the properties of space that are preserved under continuous deformations. Distinct topologies are mathematically characterized by integers called topological invariants; topologically equivalent objects, such as a donut and a coffee cup, share the same invariant (the number of "holes"). An object undergoes a topological phase transition whenever an abrupt transformation changes the topological invariant. Over the past few decades, notions of topology have become ubiquitous in materials science, culminating in the 2016 Nobel Prizes in Physics and Chemistry. The topological nature of electronic states is a pivotal concept in various recent advances in low dimensional quantum systems. This project aims to investigate ultrafast nonlinear photonic phenomena in newly discovered two-dimensional materials of the graphene family supporting topological phase transitions. The project focuses on discovery and application of fundamental material properties for controlled functionality and performance prediction beyond the linear response regime, and it will significantly advance the country's initiatives in nanotechnology and nanophotonics. Investigations on the interplay between topological chiral edge states and nonreciprocal behavior arising from nonlinearities will unveil the potential of the graphene family materials as a reliable platform for information transport, with implications for quantum computing.

Technical Outcomes

The project developed a comprehensive theory framework for describing the relation between the microscopic non-equilibrium dynamics of Dirac-like fermions in two-dimensional topological insulators and their ensuing macroscopic nonlinear processes. By bringing topological aspects to the realm of nonlinear photonics we discovered topological phase transitions (TPT) fingerprints embedded in the ultrafast response of these systems. These include time-delays in harmonic emission as well as topology dependent differences in harmonic intensity, polarization, and spectrum; all within experimental reach.

Publications

Journal Articles

Caravelli, F., B. Yan, L. Garcia-Pinto and A. Hamma. Energy storage and coherence bounds in closed and open quantum batteries. Submitted to *Quantum*. (LA-UR-20-30512)

de Melo Kort-Kamp, W. J., F. Culchac, F. Rosa, C. Farina, R. Capaz and F. Pinheiro. Harnessing the photonic local density of states in graphene Moir\xc3\xa9 superlattices. Submitted to *PRB*. (LA-UR-21-20508)

Malla, R. K., A. B. Saxena and W. J. de Melo Kort-Kamp. Emerging nonlinear Hall effect in Kane-Mele two-dimensional topological insulators. Submitted to *Physical Review B*. (LA-UR-21-28047)

Malla, R. K., V. Y. Chernyak and N. Sinitsyn. Nonadiabatic transitions in Landau-Zener grids: integrability and semiclassical theory. Submitted to *Physical Review B*. (LA-UR-21-20136)

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear photonics of topological Dirac fermions in spin-orbit coupled graphene family materials. Submitted to *Communications physics*. (LA-UR-20-30407)

Muniz, Y., A. Manjavacas, C. Farina, D. A. R. Dalvit and W. J. de Melo Kort-Kamp. Unraveling the decay mechanisms of two-quanta spontaneous photonic transitions. Submitted to *Nature Photonics*. (LA-UR-20-20456)

Muniz, Y., C. Farina and W. J. de Melo Kort-Kamp. Casimir forces in the flatland: impact of topological phase transitions and quantum Hall physics. Submitted to *Physical Review B*. (LA-UR-20-28079)

. L. L. *. C. F. *. H. A. Oliviero, S. F. and F. Caravelli. Random matrix theory of the isospectral twirling. 2021. *SciPost Physics*. **10 (3): 076. (LA-UR-20-30225 DOI: 10.21468/SciPostPhys.10.3.076)

Presentation Slides

de Melo Kort-Kamp, W. J. Ultrafast nonlinear photonics in Kane-Mele two-dimensional topological insulators. Presented at *Korean Physical Society Fall Meeting*, Online, Korea, South, 2021-10-20 - 2021-10-22. (LA-UR-21-30372)

Malla, R. K., A. B. Saxena and W. J. de Melo Kort-Kamp. Nonlinear planar Hall effect in graphene family monolayers. Presented at *APS March meeting, 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22394)

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear optical response of graphene family materials near topological phase transitions. Presented at *2020 APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21863)

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear Photonics of Topological Phase Transitions in the Graphene Family. . (LA-UR-21-23659)

Overcoming the Curse of Dimensionality to Predict Chemical Reactivity

Beth Lindquist
20180758PRD4

Project Description

This project aims to provide a critical component of an equation of state (EOS) that is typically missing from atomistic modeling. Such work will be directly applied to high explosives (HE) equation of state modeling. This can be used to understand many important issues confronting the stockpile, such as understanding and predicting the behavior and performance of HE. This will be critical for new formulations or aged HE materials.

Publications

Journal Articles

*Howard, M. P., R. B. Jadrich, B. A. Lindquist, F. Khabaz, R. T. Bonnecaze, D. J. Milliron and T. M. Truskett. Structure and phase behavior of polymer-linked colloidal gels. 2019. *The Journal of Chemical Physics*. **151** (12): 124901. (LA-UR-19-26202 DOI: 10.1063/1.5119359)

Lindquist, B. A. Connecting Inverse Design with Experimentally Relevant Models. Submitted to *Journal of Physics: Conference Series*. (LA-UR-20-21571)

*Lindquist, B. A. Inverse design of equilibrium cluster fluids applied to a physically informed model. 2021. *The Journal of Chemical Physics*. **154** (17): 174907. (LA-UR-21-21954 DOI: 10.1063/5.0048812)

*Lindquist, B. A., R. B. Jadrich, M. P. Howard and T. M. Truskett. The role of pressure in inverse design for assembly. 2019. *The Journal of Chemical Physics*. **151** (10): 104104. (LA-UR-19-25001 DOI: 10.1063/1.5112766)

*Sherman, Z. M., M. P. Howard, B. A. Lindquist, R. B. Jadrich and T. M. Truskett. Inverse methods for design of soft materials. 2020. *The Journal of Chemical Physics*. **152** (14): 140902. (LA-UR-20-20466 DOI: 10.1063/1.5145177)

Spencer, J. A., D. A. Shutt, S. Moser, H. C. Clegg, H. J. Wearing, H. Mukundan and C. A. Manore. Distinguishing Viruses Responsible for Influenza-like Illness. Submitted to *Journal of Theoretical Biology*. (LA-UR-21-27457)

Presentation Slides

Lindquist, B. A. Using Statistical Inference to Discover Interactions for Colloidal Self-Assembly. Presented at *Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23041)

Lindquist, B. A. Statistical Inference of Equilibrium Statistical Mechanical Models. Presented at *33rd Annual CSP Workshop: Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, Georgia, United States, 2020-02-17 - 2020-02-21. (LA-UR-20-21358)

Lindquist, B. A. Using Inverse Design to Facilitate Colloidal Self-Assembly. . (LA-UR-21-25905)

Lindquist, B. A. Self-Assembly of gels, clusters, and other modulated phases via a physically informed model. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, San Diego, California, United States, 2022-03-20 - 2022-03-24. (LA-UR-22-22571)

Lindquist, B. A. and R. B. Jadrich. Chemical Bonding in High Explosives. Presented at *ACS Fall 2021: Resilience of Chemistry*, Atlanta, Georgia, United States, 2021-08-22 - 2021-08-26. (LA-UR-21-28255)

A Novel "Three-in-One" Metal Organic Framework-Based Platform For Nanoparticle Encapsulation and Organization

Ekaterina Dolgopolova
20190620PRD1

Project Description

New and improved light-emitting, light-directing and light-transmitting materials are needed to support advanced technologies that underpin economic competitiveness, e.g., Information Science and Technology, as well as global security, e.g., via enabling new tools for improved Remote Sensing for Nuclear Nonproliferation and Counterproliferation, new materials for scintillation and radiation detection for Nuclear Nonproliferation and Counterproliferation, new strategies for Information Collection, Surveillance, and Reconnaissance, and new sensors/detectors for Chemical and Biological Weapons and Defense. The proposed work involves the development of novel, flexible photonic materials.

Publications

Presentation Slides

Dolgopolova, E. and J. A. Hollingsworth. Alternative plasmonic nanomaterials as building blocks for Purcell-enhanced emission in the infrared. Presented at *2020 Spring ACS National Meeting, COLL Virtual Technical Symposium*, Los Alamos, New Mexico, United States, 2020-03-22 - 2020-03-24. (LA-UR-20-22500)

Dolgopolova, E. and J. A. Hollingsworth. Alternative nanomaterials with size-dependent plasmonic properties for Purcell-enhanced emission in the infrared. Presented at *ACS Fall 2020 Virtual Meeting*, San Francisco, California, United States, 2020-08-16 - 2020-08-16. (LA-UR-20-26512)

Dolgopolova, E. and J. A. Hollingsworth. Shooting for the Stars: Opening New Dimensions for Metal-Organic Frameworks. Presented at *Center for Space and Earth Science Symposium*, Los Alamos, New Mexico, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28567)

Dolgopolova, E. and J. A. Hollingsworth. Plasmonic spinel oxide nanocrystals afford Purcell-enhanced emission in the infrared. Presented at *ACS Spring 2021*, Online, New Mexico, United States, 2021-04-04 - 2021-04-30. (LA-UR-21-23397)

Dolgopolova, E. and J. A. Hollingsworth. Controlled growth of metal-organic frameworks in gels. Presented at *ACS Spring Meeting 2021*, Online, New Mexico, United States, 2021-04-04 - 2021-04-30. (LA-UR-21-23396)

Posters

Dolgopolova, E., D. Li, J. D. Watt, G. Pilania, C. Ocampo, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Alternative Plasmonic Nanomaterials for Purcell-Enhanced Emission in the Infrared Region. Presented at *CINT Annual Meeting*, Online, New Mexico, United States, 2020-09-21 - 2020-09-24. (LA-UR-20-27165)

Dolgopolova, E., J. S. Mohar, Y. Kim, G. Pilania, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Semiconductors Helping Semiconductors: Alternative Plasmonic Nanomaterials as Building Blocks for Purcell-enhanced Emission. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29475)

Novel X-ray Imaging to Unlock the Potential of Antiferromagnetic Materials

Adra Carr
20190623PRD2

Project Description

This research will help to develop techniques critical to understanding how materials structure at the nanometer scale controls its magnetic and electronic behavior. Understanding this critical information is key to unlocking the potential for new magnetic materials that could have broad impact in information systems technology (computers, cell phones, sensors, etc). Understanding how our information systems behave is critical to all aspects of our modern life including commerce and national security.

Publications

Journal Articles

Carr, A. V., J. M. Bowlan, C. Mazzoli, A. Barbour, W. Hu, S. Wilkins, C. Walker, X. Ding, N. Lee, J. H. Kim, Y. J. Choi, S. Lin, R. L. Sandberg and V. Zapf. Evidence for the Alternating Next-Nearest Neighbor model in the dynamic behavior of a frustrated antiferromagnet. Submitted to *Physical Review Letters*. (LA-UR-20-24289)

Presentation Slides

Carr, A. V., J. M. Bowlan, S. Lin, C. Mazzoli, A. Barbour, W. Hu, S. Wilkens, X. Ding, N. Lee, J. H. Kim, Y. J. Choi, R. L. Sandberg and V. Zapf. Traversing the "Devil's Staircase": Dynamic behavior of a frustrated antiferromagnet. Presented at *NSLS-II Friday Virtual Lunchtime Seminar Series (Webinar)*, Upton, New York, United States, 2020-12-04 - 2020-12-04. (LA-UR-20-29864)

Carr, A. V., V. Zapf, D. A. Yarotski and R. L. Sandberg. LDRD Project Visit: Novel X-ray Imaging to Unlock the Potential of Antiferromagnetic Materials. Presented at *LDRD Project visit*, Los Alamos, New Mexico, United States, 2020-12-14 - 2020-12-14. (LA-UR-20-30200)

Posters

Burdet, N. G., A. V. Carr, J. M. Bowlan, K. M. Mertes, J. D. Nguyen, R. Tobey, X. Ding, S. Lin, C. S. Walker, B. A. Pound, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins , V. Zapf, C. Mazzoli and R. L. Sandberg. Towards spatially mapping domain dynamics in Antiferromagnetic materials with soft x-ray scattering at NSLS-II. Presented at *SLAC Users Meeting*, Standford, California, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-25092)

Synthesis of Platinum-Rare Earth Intermetallic Fuel Cell Catalysts

Jacob Spendelow
20190640PRD3

Project Description

The project seeks to develop improved fuel cell catalysts. Fuel cells are relevant and important to multiple Department of Energy missions related to energy security, as well as fuel cells for National Nuclear Security Administration-specific national security applications. If successful, we expect that catalysts developed through this project could have transformative impact on fuel cell technology, providing near-term as well as long-term benefits for energy security and national security applications.

Publications

Journal Articles

Qiao, Z., C. Li, C. Wang, S. Hwang, B. Li, Y. Zeng, A. J. Kropf, C. E. Wegener, Q. Gong, G. Wang, D. Myers, J. Xie, J. S. Spendelow and G. Wu. Synergistic PGM-free Single Metal Sites for Promoting PtCo Ordered Intermetallic Fuel Cell Catalysts: Performance and Durability Improvements. Submitted to *Energy & Environmental Science*. (LA-UR-21-23020)

*Wang, C. and J. S. Spendelow. Recent Developments in Pt-Co catalysts for PEM Fuel Cells. 2021. *Current Opinion in Electrochemistry*. 100715. (LA-UR-20-25517 DOI: 10.1016/j.coelec.2021.100715)

*Zhao, X., C. Xi, R. Zhang, L. Song, C. Wang, J. S. Spendelow, A. I. Frenkel, J. Yang, H. L. Xin and K. Sasaki. High-Performance Nitrogen-Doped Intermetallic PtNi Catalyst for the Oxygen Reduction Reaction. 2020. *ACS Catalysis*. **10** (18): 10637-10645. (LA-UR-20-26461 DOI: 10.1021/acscatal.0c03036)

Presentation Slides

Wang, C. Intermetallic PtCo Catalysts with Enhanced Performance and Stability. . (LA-UR-21-23654)

Wang, C., D. Li, Y. S. Kim and J. S. Spendelow. Carbon Effect on the Synthesis and MEA Performances of L10 CoPt Intermetallic Catalysts. Presented at *236th Electrochemical Society Meeting*, Atlanta, Georgia, United States, 2019-10-13 - 2019-10-18. (LA-UR-19-30298)

Wang, C., Z. Qiao, V. B. Kumar, D. A. Cullen, D. Li, K. L. More, G. Wu, Y. S. Kim and J. S. Spendelow. Size-Controlled Synthesis of L10-CoPt Intermetallic Fuel Cell Catalysts on Nitrogen-Doped Mesoporous Graphitized Carbon Support. Presented at *237th Electrochemical Society Meeting*, Montreal, Canada, 2020-05-10 - 2020-05-15. (LA-UR-19-32027)

Designing New Ferroelectric Materials with Spin Crossover Transitions

Wanyi Nie
20190647PRD3

Project Description

The successful demonstration in this project will provide materials for quantum information processing and energy efficient device operation. It will provide new solution for enhancing the information security and energy security missions. Since we are expecting new physical principles in the new material systems, the outcome can lead to high impact results that push the quantum information processing forward under practical operational conditions.

Publications

Journal Articles

Owczarek, M. T., M. Lee, V. Zapf, W. Nie and R. Jakubas. Accessing one-dimensional chains of halogenoindates(III) in organic-inorganic hybrids. Submitted to *Inorganic Chemistry*. (LA-UR-22-20744)

Owczarek, M. T., P. Szklarz and R. Jakubas. Towards ferroelectricity-inducing chains of halogenoantimonates(iii) and halogenobismuthates(iii). 2021. *RSC Advances*. **11** (29): 17574-17586. (LA-UR-20-28039 DOI: 10.1039/D0RA10151F)

Presentation Slides

Owczarek, M. T., M. Lee, W. Nie and V. Zapf. Spin state transitions as a route to magnetoelectric coupling. Presented at *17th International Conference on Molecule Based Magnets*, Manchester, United Kingdom, 2021-06-14 - 2021-06-18. (LA-UR-21-25417)

Owczarek, M. T., M. Lee, W. Nie and V. Zapf. Close-to-room-temperature magnetoelectric coupling in a molecule-based material. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-02-18. (LA-UR-22-21580)

The Optoelectronic Device Applications of 2-Dimensional Interlayer Moiré Excitons

Han Htoon
20190648PRD3

Project Description

Light emitting diodes (LEDs) and lasers lie at the heart of almost all modern technologies. They make high speed internet possible and can be found inside of your television set. This project aims toward developing a new class of ultra-compact and efficient light emitting diodes and lasers by exploiting a novel phenomenon called Moire inter-layer exciton emerged at the interface of two atomically thin semiconductor layers. The devices that could be as thin as 4 atomic layers, can be fabricated by simply stacking different type of atomically thin metallic (graphene) and semiconductor layers in a way similar to Lego blocks. They can also be integrated into existing Silicon-based electronic and photonic integrated circuits. This project therefore has a potential to revolutionize telecommunication, display and flexible electronic industries.

Publications

Journal Articles

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

P. M. T. *. Z. Y. *. H. H. Zhao, H. *., H. Zhao, M. T. Pettes, Y. Zheng and H. Htoon. Site-controlled telecom-wavelength single-photon emitters in atomically-thin MoTe2. 2021. *Nature Communications*. **12** (1): 6753. (LA-UR-21-23958 DOI: 10.1038/s41467-021-27033-w)

Defect tolerant scintillators: Linking structure and performance via machine learning (ML)

Anjana Talapatra
20190656PRD4

Project Description

Nuclear processes are associated with the emission of high energy particles capable of ionizing atoms, and detecting this ionization enables the observation of the nuclear process itself and is critical for identifying nuclear materials. One such detection technique is the use of scintillators - materials that convert the energy deposited by incident radiation into visible or ultraviolet photons. However, this irradiation introduces damage in the material, lowering efficiency. This proposal aims to minimize the detrimental effect of defects by tailoring the chemistry of scintillator materials, allowing one to design defect tolerant scintillators that can absorb and nullify the adverse consequences of defects. This will be facilitated via atomistic calculations and machine learning (ML). This work will integrate first-principle calculations, experimental data and ML in line with the Materials Genome Initiative and the laboratory's Science of Signatures and Materials for the Future Science Pillars. Concomitantly, we will develop a fundamental understanding of the relationship between defects and the performance of scintillators which will be applicable to other optical materials as well. New defect-tolerant detector materials will enhance the mission-driven science at both current and future facilities and also impact other arenas such as global security, non-destructive testing and medical imaging.

Publications

Journal Articles

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. A Machine Learning Approach to Prediction of Formability and Thermodynamic Stability of Single and Double Perovskite Oxides. Submitted to *Chemistry of Materials*. (LA-UR-20-25347)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Band gap predictions of Novel Double Perovskite Oxides using Machine Learning. Submitted to *Chemistry of Materials*. (LA-UR-21-28459)

Talapatra, A. A., B. P. Uberuaga, C. R. Stanek and G. Pilania. Supporting Information: Band gap predictions of Novel Double Perovskite Oxides using Machine Learning. Submitted to *Chemistry of Materials*. (LA-UR-21-28478)

Talapatra, A. A., D. Ghosh, B. P. Uberuaga and G. Pilania. Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. 2021. *Journal of Materials Science*. **56** (28): 15812-15823. (LA-UR-21-23719 DOI: 10.1007/s10853-021-06294-2)

Presentation Slides

Talapatra, A. A. A Machine-Learning based Hierarchical Screening Strategy to Expedite Search of Novel Scintillator Chemistries. Presented at *MRS Fall Meeting, 2019*, Boston, Massachusetts, United States, 2019-12-01 - 2019-12-06. (LA-UR-19-31946)

Talapatra, A. A. A Machine Learning Guided Discovery of Novel Oxide Perovskites for Scintillator Applications. Presented at *TMS 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-22212)

Talapatra, A. A. Accelerating scintillator materials discovery using Machine Learning. . (LA-UR-21-24920)

Talapatra, A. A. A Machine Learning aided hierarchical screening strategy for materials discovery. . (LA-UR-21-27531)

Talapatra, A. A. A Machine-learning Based Hierarchical Framework to Discover Novel Scintillator Chemistries. Presented at *Materials Science & Technology (MS&T 2021)*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-20. (LA-UR-21-30152)

Uberuaga, B. P. Highlights performed on LANL IC on the project w19_matprops. . (LA-UR-21-24026)

Other

Talapatra, A. A. A Machine Learning aided hierarchical screening strategy for materials discovery. Audio/Visual. (LA-UR-21-27864)

Development of Next Generation Microstructure-aware Burn Models for High Explosives.

Tariq Aslam
20190658PRD4

Project Description

The main task is to develop high-fidelity microstructure models to comprehensively understand the physics of energy-localization, reaction initiation and growth at the grain-scale of High Explosives materials. The end goal is to develop a materials-by-design facility that can be used for the design of precisely controlled energy-delivery systems.

Publications

Journal Articles

Rai, N. K. and T. D. Aslam. Evaluation of the Thermodynamic Closure Models for Partially Reacted Two-Phase Mixture of Condensed Phase Explosives. Submitted to *Journal of Applied Physics*. (LA-UR-21-31716)

Presentation Slides

Rai, N. K. Next Generation Microstructure-Aware Burn Models for High Explosives. . (LA-UR-21-24186)

Importance of Metal/Oxide Interfaces to Design and Tailor Composite Material Properties.

Blas Uberuaga
20200676PRD1

Project Description

Materials are at the heart of energy technologies that have the potential for alleviating many of our current societal challenges, from climate change to energy security. The ability to tune material properties grows exponentially when we can mix materials of two very different natures, such as a metal with an insulating oxide. However, this mixing inevitably leads to interfaces between the two materials, which can have a dramatic impact on the defects that dictate the properties of the material. By examining these interfaces and interrogating the ways in which the interfaces impact defects, we will build a fundamental understanding of this interaction that can then be used in the design of new materials with enhanced functionality for radiation and/or corrosion environments, battery technologies, and catalytic applications. These areas are central to the core mission of Department of Energy.

Publications

Journal Articles

*Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Critical Assessment of the Thermodynamics of Vacancy Formation in Fe2O3 Using Hybrid Density Functional Theory. 2020. *The Journal of Physical Chemistry C*. **124** (43): 23988-24000. (LA-UR-20-24936 DOI: 10.1021/acs.jpcc.0c07522)

*Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Interplay between defect transport and cation spin frustration in corundum-structured oxides. 2021. *Physical Review Materials*. **5** (3): 034410. (LA-UR-20-28924 DOI: 10.1103/PhysRevMaterials.5.034410)

Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Correction to "Critical Assessment of the Thermodynamics of Vacancy Formation in Fe2O3 Using Hybrid Density Functional Theory". Submitted to *Journal of Physical Chemistry C*. (LA-UR-21-20017)

Yano, K. H., A. A. Kohnert, A. Banerjee, D. J. Edwards, E. F. Holby, T. C. Kaspar, H. Kim, T. G. Lach, S. D. Taylor, Y. Wang,

B. P. Uberuaga and D. K. Schreiber. Radiation-Enhanced Anion Transport in Hematite. Submitted to *Chemistry of Materials*. (LA-UR-20-28988)

Presentation Slides

Banerjee, A., A. A. Kohnert, E. F. Holby and B. P. Uberuaga. Interplay between defect transport and cation spin frustration in corundum-structured oxides. Presented at *MRS 2021 Virtual Spring Conference*, Los Alamos, New Mexico, United States, 2021-04-17 - 2021-04-23. (LA-UR-21-24006)

Strain Susceptibility of Quantum Critical Fluctuations

Johanna Palmstrom
20200680PRD1

Project Description

Electronic properties of materials can be strongly affected by applied stress. This project focuses on understanding the mechanism behind unconventional (high temperature) superconductors by measuring their electronic responses to strain in extremely high magnetic fields. There are two main goals: to develop methods of applying different symmetry strains that are compatible with pulsed magnetic field environments, and to gain a better understanding of exotic mechanisms of superconductivity. Long term, understanding superconductivity will lead to favorable material properties for quantum information processing, energy transmission and storage. Increasing the operating temperature and density of stored energy could lead to viable large-scale superconducting energy storage as an important complement to alternative energy sources. In addition, this measurement technique would be applicable to study phase transitions in a wide range of 'mission relevant' materials under extreme conditions. For example, actinide materials can be tuned with pressure through a variety of phase transitions, making them excellent candidate materials for strain measurements. In particular, plutonium (Pu) exhibits many structural phases and phase transitions which are not fully understood and measurements of the symmetry resolved strain susceptibility will give insights into the nature of these phase transitions.

Publications

Journal Articles

Palmstrom, J. C., P. Walmsley, J. A. W. Straquadine, M. E. Sorensen, S. T. Hannahs, D. H. Burns and I. R. Fisher. Comparison of temperature and doping dependence of elastoresistivity near a putative nematic quantum critical point. Submitted to *Nature Communications*. (LA-UR-22-20372)

Reports

Palmstrom, J. C. 20200680PRD1 Data Sheet. Unpublished report. (LA-UR-21-25761)

Palmstrom, J. C. Exploring Topological Phase Transitions in Dirac Semimetals. Unpublished report. (LA-UR-22-21037)

Presentation Slides

Palmstrom, J. C. Elastoresistivity of Fe-based Superconductors in High Magnetic Fields. Presented at *ARHMF2020 & KINKEN Materials Science School 2020 for Young Scientists*, Internet, Japan, 2020-12-01 - 2020-12-03. (LA-UR-20-29887)

Palmstrom, J. C. LDRD Project 20200680PRD1: Strain Susceptibility of Quantum Critical Fluctuations. Presented at *LDRD Project Visit*, Los Alamos, New Mexico, United States, 2021-05-13 - 2021-05-13. (LA-UR-21-24490)

Palmstrom, J. C. Strain as a Controllable Tuning Parameter: An in-situ Method to Break Crystal Symmetries and Change Material Properties. Presented at *Science in 3*, Los Alamos, New Mexico, United States, 2021-09-01 - 2021-09-01. (LA-UR-21-26711)

Palmstrom, J. C. High Field Elastoresistivity Measurements of Quantum Materials. Presented at *NSF site visit*, Los Alamos, New Mexico, United States, 2021-07-27 - 2021-07-27. (LA-UR-21-26712)

Electrically Pumped Laser Diodes Using Charged Colloidal Quantum Dots

Victor Klimov
20200685PRD2

Project Description

If realized, solution-processable, electrically pumped lasers (or "laser diodes") can revolutionize numerous technologies including optoelectronics, telecommunication, medical diagnostics, and homeland security. This project proposes that this challenge can be successfully tackled using specially engineered colloidal quantum dots (QDs) incorporated into "current-focusing" light emitting diodes (LED). The proposed research takes advantage of a series of recent accomplishments of Physical Chemistry Applied Spectroscopy (C-PCS) researchers that includes demonstration of QD optical gain with electrical pumping and the development of dual-function optically pumped laser/LED devices. This project's objective is to build upon these advances and demonstrate a functional QD laser diode, which will be the first practically realized solution-processable laser operating under electrical excitation. This project will apply an integrated approach: boost current density by employing a "current-focusing" LED design with short-pulse electrical pumping; enable lasing action by integrating a distributed feedback cavity into the transparent LED electrode; and enhance modal gain of a QD layer by enhancing the field confinement factor by carefully engineering a refractive-index profile across the device stack. The ultimate result of this integrated effort will be the first-ever solution-processable laser diode.

Publications

Presentation Slides

Ahn, N. and V. I. Klimov. Electrically pumped laser diodes using charged quantum dots. Presented at *LDRD project visit*, Los alamos, New Mexico, United States, 2021-01-11 - 2021-01-11. (LA-UR-21-20472)

Design and Discovery of Novel, Two-Dimensional f-electron Quantum Materials

Eric Bauer
20200686PRD2

Project Description

This project will discover new two-dimensional rare earth and actinide quantum materials and investigate their novel and interesting quantum states. Quantum materials have great potential for use in future architectures for quantum computing and quantum information science to ensure the Nation's energy security.

Publications

Journal Articles

*Liu, Y., Z. Hu, M. Abeykoon, E. Stavitski, K. Attenkofer, E. D. Bauer and C. Petrovic. Polaronic transport and thermoelectricity in single crystals. 2021. *Physical Review B*. **103** (24): 245122. (LA-UR-21-25285 DOI: 10.1103/PhysRevB.103.245122)

Atomistic Modeling and Machine Learning for Bio-advantaged Polymer Design

Ghanshyam Pilania
20200688PRD2

Project Description

Plastics are ubiquitous and plastic pollution is currently being considered as one of the largest environment threats. To address this challenge, current research efforts are focused on developing new bio-degradable and bio-compatible polymers which have the potential to replace petroleum-based plastics for a sustainable future. Bio-derived polymers offers a faster degradation; however, they suffer from poor mechanical and elastic properties and high cost of production. To mitigate this shortcoming, this project aims at understanding design rules for improved polymer hybrid materials which combine bio-based chemistries with conventional polymers to achieve the desired favorable combination of functional properties without compromising much on the biodegradability. The main goal of this project is to develop a knowledge base of design rules and to discover, design, and develop new hybrid bio-degradable polymers via combining conventional and bio-advantaged polymers—will enable a more cost-effective, smooth and sustainable path to replace petroleum-based products with sustainable bio-based alternatives. The research is well aligned with the Department of Energy's mission in Clean Energy Innovation. The improved ability to develop eco-friendly bioplastics will lead to a reduced carbon footprint for plastics manufacturing, and innovative solutions to reduce the accumulation and persistence of plastics in the environment.

Publications

Journal Articles

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Glass Transition Temperature Predictions of Binary Copolymers and Blends of Polyhydroxyalkanoate Biopolymers: Compositional and Configurational Dependence. Submitted to *Macromolecules*. (LA-UR-20-30478)

Bejagam, K. K., N. S. Gupta, K. Lee, C. N. Iverson, B. L. Marrone and G. Pilania. Predicting the Mechanical Response of Polyhydroxyalkanoate Biopolymers Using Molecular Dynamics Simulations. Submitted to *Polymers*. (LA-UR-21-32062)

Presentation Slides

Bejagam, K. K. In the quest for "Green Polymers". Presented at *CPMU Silver Jubliee meeting*, Bangalore, India, 2020-12-18 - 2020-12-18. (LA-UR-20-30343)

Bejagam, K. K. Atomistic Modeling and Machine Learning for Bio-advantaged Polymer Design. . (LA-UR-21-29152)

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Computational aided design of bio-polymers by mining the PHA chemical space. Presented at *ACS spring Meeting 2021*, Los Alamos, New Mexico, United States, 2021-04-05 - 2021-04-16. (LA-UR-21-23600)

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Design of Bio-Polymers by Mining the PHA Chemical Space. Presented at *International Conference on Biopolymers and Bioplastics*, Los Alamos, New Mexico, United States, 2021-06-21 - 2021-06-22. (LA-UR-21-26177)

Highly Ordered Refractory Intermetallics: the ZIA-Phases Project

Stuart Maloy
20200689PRD2

Project Description

In this research, we propose to investigate a new class of materials, Zigzag Intermetallic Advanced Phases (ZIA) for high dose nuclear applications. We will fabricate, characterize and test these materials using high dose ion irradiation. These novel materials may have numerous nuclear reactor applications especially for use in new advanced reactors such as microreactors and Gen IV reactors such as the sodium or lead fast reactors as well as potential fusion reactor applications which have direct application to the energy security mission at Los Alamos National Lab.

Publications

Journal Articles

Flei\xc3\x9fner-Rieger, C., M. A. Tunes, C. Gammer, T. J \xc3\xb6rg, P. Pfeifer, M. Musi, F. Mendez-Martin, H. Clemens and S. Mayer. On the existence of orthorhombic martensite in a near-\xce\xb1 titanium base alloy used for additive manufacturing. 2021. *Journal of Alloys and Compounds*. 163155. (LA-UR-21-28594 DOI: 10.1016/j.jallcom.2021.163155)

Iroc, L., O. El Atwani, M. A. Tunes, Y. Kalay and E. Aydogan. Enhancement of the strength-ductility trade-off by transformation-induced nanolamellar structures and nanotwinning in oxygen-doped TiZrHfNbTa refractory high-entropy alloys. Submitted to *Advanced Materials*. (LA-UR-22-21273)

P. Ramirez, O. M., M. A. Tunes, M. M. Mennucci, M. Starykevich, C. Neves, M. G. S. Ferreira, S. Pogatscher and H. G. de Melo. Corrosion behaviour of tartaric-sulfuric acid anodized AA2024-T3 post-treated in Ce- containing solutions. Submitted to *Acta Materialia*. (LA-UR-22-20081)

Stemper, L., M. A. Tunes, R. Tosone, P. Uggowitzer and S. Pogatscher. On the potential of aluminum crossover alloys. 2021. *Progress in Materials Science*. 100873. (LA-UR-21-25169 DOI: 10.1016/j.pmatsci.2021.100873)

Tunes, M. A., O. El Atwani, G. Greaves, P. D. Rack, W. L. Boldman, C. G. Sch\xc3\xb6n, S. Pogatscher, S. A. Maloy and Y. Zhang. Irradiation stability and induced ferromagnetism in a nanocrystalline CoCrCuFeNi highly-concentrated alloy. 2021. *Nanoscale*. **13** (48): 20437-20450. (LA-UR-21-22885 DOI: 10.1039/D1NR04915A)

Presentation Slides

Tunes, M. A. A brief history of the electronic friendship between H and Zr. Presented at *Dr. Tarik Saleh group*, Los Alamos, New Mexico, United States, 2021-06-10 - 2021-06-10. (LA-UR-21-25482)

Design and Discovery of Novel High-entropy Alloys

Saryu Fensin
20200755PRD3

Project Description

There is a need to develop materials that can withstand extreme mechanical and thermal extremes. Currently, development of many applications are limited by the availability of such materials. However, recent development of a new class of materials termed high entropy alloys provides hope as these possess a unique combination of high strength and ductility. These are metal alloys with multiple chemical elements that are combined in a specific way. Minor changes in the composition of the elements that make up these alloys can alter the material properties drastically. The combination of elements that can be used to manufacture these alloys are numerous. Hence, discovery of alloys can be time consuming. The objective of this project is to couple modeling and experiments to facilitate rapid discovery of alloys. Unlike the rest of the field using atomistic level simulations for materials discovery, we will perform high throughput manufacturing of these materials coupled with rapid characterization that will be used to generate a database. This database will then be an input to machine learning tools. This will provide us the capability to develop materials with tailored properties that will be indispensable to various projects within the National Nuclear Security Administration.

Publications

Journal Articles

*Lattice-Distortion-Enhanced Yield Strength in a Refractory High-Entropy Alloy. 2020. *Advanced Materials*. **32** (49): 2004029. (LA-UR-20-27498 DOI: 10.1002/adma.202004029)

Investigation of phase-transformation path in TiZrHf(VNbTa)x refractory high-entropy alloys and its effect on mechanical property. 2021. *Journal of Alloys and Compounds*. **886**: 161187. (LA-UR-21-25855 DOI: 10.1016/j.jallcom.2021.161187)

S. G. *. G. M. C. *. O. L. *. A. K. *. F. S. J. *. L. P. K. Lee, C. *., C. Lee and S. J. Fensin. Effects of Zr addition on lattice strains and electronic structures of NbTaTiV high-entropy alloy. 2022. *Materials Science and Engineering: A*. **831**: 142293. (LA-UR-22-20347 DOI: 10.1016/j.msea.2021.142293)

*Lee, C., F. Maresca, R. Feng, Y. Chou, T. Ungar, M. Widom, K. An, J. D. Poplawsky, Y. Chou, P. K. Liaw and W. A. Curtin. Strength can be controlled by edge dislocations in refractory high-entropy alloys. 2021. *Nature Communications*. **12** (1): 5474. (LA-UR-21-22188 DOI: 10.1038/s41467-021-25807-w)

Lee, C., J. Brechtl and P. K. Liaw. Research on Bulk-metallic Glasses and High-entropy Alloys in Peter K. Liaw's Group and with His Colleagues. Submitted to *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*. (LA-UR-20-30049)

*Lee, C., J. Kim, S. J. Hong, J. K. Lee, K. B. Kim, J. H. Lee, J. Han and G. Song. Development of coherent-precipitate-hardened high-entropy alloys with hierarchical NiAl/Ni2TiAl precipitates in CrMnFeCoNiAlxTiy alloys. 2021. *Materials Science and Engineering: A*. **823**: 141763. (LA-UR-21-26983 DOI: 10.1016/j.msea.2021.141763)

Presentation Slides

Lee, C., G. Kim, Y. Chou, B. L. Musico, M. C. Gao, K. An, G. Song, Y. Chou, V. Keppens, W. Chen and P. K. Liaw. Unique Deformation Behavior in the NbTaTiV Refractory High entropy Alloy. Presented at *TMS 2021 Annual Meeting and Exhibition*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21922)

Lee, C., G. Kim, Y. Chou, M. C. Gao, K. An, G. Song, Y. Chou, W. Chen, S. J. Fensin and P. K. Liaw. Deformation Behavior in the Refractory High-entropy Alloys. Presented at *MS&T21*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-21. (LA-UR-21-30168)

Lee, C., G. Song, M. C. Gao, W. Chen, K. An, L. Ouyang and P. K. Liaw. Distinctive Room Temperature Deformation Behavior in Plastic BCC Refractory High-entropy Alloys. Presented at *TMS 2021 Annual Meeting and Exhibition*, Virtual, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21902)

Lee, C., N. Li and S. J. Fensin. Design and Development of Strong and Ductile Single BCC Refractory High-entropy Alloys for Elevated-Temperature Applications. Presented at *Department Seminar at New Mexico Institute of Mining*

and Technology, Socorro, New Mexico, United States, 2022-02-11 - 2022-02-11. (LA-UR-22-21042)

Lee, C., Y. Chou, G. Kim, M. C. Gao, K. An, J. Brechtl, C. Zhang, W. Chen, J. Poplawsky, G. Song, Y. Ren, Y. Chou, N. Li, S. J. Fensin and P. K. Liaw. Lattice Distortion in Refractory High-entropy Alloys. Presented at *2021 Virtual MRS Spring Meeting & Exhibit*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-23. (LA-UR-21-23819)

Topological Superconductivity in Van Der Waals Materials as a Platform for Qubits

Christopher Lane
20200756PRD3

Project Description

In December 2018, the National Quantum Initiative (NQI) Act was signed into law to speed up the advancement of quantum related technology and quantum computing. The Department of Energy is expected to invest heavily in materials science for quantum information processing in the next five years, including the National Quantum Information Science Research Centers. By performing simulations based on the coherent superposition of quantum states, quantum computers hold huge promise to transform our society by solving tough problems intractable on our classical computers built with on-off bit technology. The grand challenge facing the quantum computers is the overhead from the error correction needed to combat the decoherence. Therefore, quantum bits with long coherence time are desirable. This project directly addresses this challenge by searching and identifying the topological superconductivity in two-dimensional transition-metal dichalcogenides and their heterostructures. Topological superconductors are believed to host the exotic quasiparticles, the so called Majorana fermion modes. The quantum bits built upon these exotic particles will enable fault-tolerant quantum computation that is immune to conventional decoherence sources. Success from this project will provide a fundamental understanding and design principles of topological superconductivity, paving the way for robust quantum information platforms.

Publications

Journal Articles

Huang, Z., C. A. Lane, D. A. Yarotski, A. J. Taylor and J. Zhu. Topological superconducting domain walls in magnetic Weyl semimetals. Submitted to *Physical Review Letters*. (LA-UR-21-25206)

Lane, C. A., L. Chen, H. Hu, E. Nica, J. Zhu and Q. Si. Multiorbital spin-triplet pairing and spin resonance in the heavy fermion superconductor UTe2. Submitted to *Physical Review Letters*. (LA-UR-21-32485)

Markiewicz, R. S., B. Singh, C. A. Lane and A. Bansil. High-order Van Hove singularities in cuprates and related high-Tc superconductors. Submitted to *Nature Communications*. (LA-UR-21-22462)

Matt, C. E., Y. Liu, H. Pirie, N. Drucker, N. H. Jo, B. Kuthanazhi, Z. Huang, C. A. Lane, S. L. Bud'Ko, J. Zhu, P. C. Canfield and J. E. Hoffman. Spin-polarized imaging of strongly interacting fermions in the ferrimagnetic state of Weyl candidate CeBi. Submitted to *Physical Review Letters*. (LA-UR-20-28429)

Peng, S., C. A. Lane, Y. Hu, M. Guo, X. Chen, M. Matzelle, Z. Sun, M. Hashimoto, D. H. Lu, Z. X. Shen, T. Wu, X. H. Chen, R. S. Markiewicz, Y. Wang, A. Bansil, S. D. Wilson and J. F. He. Electronic nature of the pseudogap in electron-doped Sr2IrO4. Submitted to *Nature Physics*. (LA-UR-20-26487)

Setty, C., C. A. Lane, L. Chen, H. Hu, J. Zhu and Q. Si. Electron correlations and charge density wave in the topological kagome metal FeGe. Submitted to *Physical Review Letters*. (LA-UR-22-21964)

Winter, G., M. Matzelle, C. A. Lane and A. Bansil. Fully-Compensated Ferrimagnetic Spin Filter Materials within the CrMNAl Equiatomic Quatnernary Heusler Alloys. Submitted to *Journal of Applied Physics*. (LA-UR-20-28904)

Zhang, R., C. A. Lane, B. Singh, J. Nokelainen, B. Barbiellini, R. S. Markiewicz, A. Bansil and J. Sun. f-electron and magnetic ordering effects in nickelates LaNiO2 and NdNiO2: remarkable role of the cuprate-like 3dx2–y2 band. Submitted to *npj Quantum Materials*. (LA-UR-20-27054)

Presentation Slides

Lane, C. A. and J. Zhu. Identifying Topological Superconductivity in the 2D Transition Metal Dichalcogenides. Presented at *APS March Meeting 2021*, los alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22432)

Matzelle, M., C. A. Lane, R. He, R. S. Markiewicz and A. Bansil. An ab initio Study of Oxygen Vacancies in Ba2CuO3+\xce \xb4. Presented at *APS March Meeting 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22472)

Ning, J., C. A. Lane, M. Matzelle, B. Singh, B. Barbiellini, R. S. Markiewicz, A. Bansil and J. Sun. Accurate lattice dynamics

of cuprates from first principles. Presented at *APS March Meeting 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22479)

Zhu, J. Dark Matter Detection with Strongly Correlated Topological Matter: Flatband Effect. Presented at *Quantum Matter & Beyond*, Jacksonville Beach, Florida, United States, 2021-12-15 - 2021-12-17. (LA-UR-21-32248)

Zhu, J. Dark Matter Detection with Strongly Correlated Topological Matter: Flatband Effect. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21944)

Zhu, J. and C. A. Lane. Density functional theory (DFT): A Primer. . (LA-UR-21-30165)

Synthesis and Stabilization of 2D Electrenes as Novel Nanoscale Magnets

Sergei Ivanov
20200776PRD4

Project Description

Electrides are ionic crystals wherein unbound electrons act as anions filling voids between inorganic cations in the crystal structure. The differing dimensionality of the void space results in varying electronic or magnetic properties, which is further expanded when approaching the nanoscale. When electrides are prepared as 2-Dimensional (2D) nanosheets, i.e. electrenes, the unbound electron is still retained having potential uses in spintronic, negative refractive index, and superconductor applications. This project aims to develop new synthetic protocols for electride materials to avoid the use of solid state reactions which are energy and time intensive. The success of this endeavor will result in a streamlined methodology that will result in the easy access of this exotic material for the study and development of its properties for its eventual use in quantum science. The National Quantum Initiative (of which the Department of Energy is an "integral partner") has identified 2D materials as a key platform to realize quantum information science & technology; both the range of accessible material properties and the 2D nature of electrenes make this system an important, yet relatively unexplored, 'building block' quantum information, science and technology (QIS&T) material where Los Alamos National Laboratory could take the lead.

Multi-scale Visualization for Tuning High-efficiency and Low-catalyst-loading

Ulises Martinez
20200777PRD4

Project Description

This projects seeks to develop a new Los Alamos National Laboratory capability which will directly impact the design and development of new electrode structures for electrochemical energy storage and conversion devices such as electrolyzers and fuel cells. Electrolyzers and fuel cells are relevant and important to multiple Department of Energy (DOE) missions related to energy security, including DOE's Earthshots Initiative. Successful development of this novel technique will be transformative, significantly impacting the design of new electrode structures for energy-related electrochemical devices with improved performance and durability, providing near-term as well as long-term benefits for energy security and national security applications.

Publications

Presentation Slides

Yang, G. Structured Membrane-electrode Interface for Highly Efficient PEM Fuel Cell. . (LA-UR-21-22645)

Characterizing the Spatial and Temporal Evolution of Nuclear Materials during Coupled Irradiation and Corrosion

Nan Li
20210760PRD1

Project Description

The goal of this project is to develop a novel in situ testing devices to study materials response at a coupled corrosion and irradiation extremes. This proposal seeks to identify the underlying principles that control material expression in extreme environments by conducting in situ (i.e. with irradiation at the same time) diagnostic testing on corrosion mechanisms in nuclear-relevant materials. Outstanding scientific questions in this field include how complex oxides grow in extreme environments and how irradiation effects the overall corrosion behavior of materials. To solve these questions and, more importantly, to inform the design of materials that better withstand degradation in this environment of coupled extremes, in situ characterization of the temporal and spatial development of complex oxides on metallic materials is needed.

Publications

Journal Articles

Derby, B. K., S. Mills, S. Agarwal, J. A. Valdez, J. K. S. Baldwin, M. M. Schneider, A. Minor, B. P. Uberuaga, F. A. Selim and N. Li. Microstructural Dependence of Defect Formation in Iron-Oxide Thin Films. Submitted to *Applied Surface Science*. (LA-UR-21-31255)

Derby, B. K., Y. Sharma, J. A. Valdez, M. R. Chancey, Y. Wang, E. L. Brosha, D. J. Williams, M. M. Schneider, A. Chen, B. P. Uberuaga, C. Kreller and M. T. Janish. Interfacial cation mixing and microstructural changes in bilayer GTO/GZO thin films after irradiation. Submitted to *Journal of Materials*. (LA-UR-22-21386)

Paudel, B., Y. Sharma, B. K. Derby, G. Pilania, M. M. Schneider, A. C. Jones, H. Nakotte, M. T. Pettes and A. Chen. Effect of lattice strain on magnetism in epitaxial YCrO3 films. 2022. *Materials Research Letters*. **10** (1): 29-35. (LA-UR-21-30206 DOI: 10.1080/21663831.2021.2010822)

Presentation Slides

Derby, B. K., C. Kreller and M. T. Janish. Interfacial cation mixing and microstructural changes in bilayer GTO/GZO thin films after irradiation. Presented at *Minerals, Metals & Materials Society (TMS) Annual Meeting and Exhibition*, Anaheim, California, United States, 2022-02-28 - 2022-03-03. (LA-UR-22-21547)

Derby, B. K., E. Lang, T. Clark, K. Hattar, J. Han, C. Kreller, M. T. Janish and N. Li. Characterizing the Spatial and Temporal Evolution of Iron Thin Films During Coupled Irradiation and Corrosion. Presented at *MS&T 2021*, Columbus, Ohio, United States, 2021-10-17 - 2021-10-17. (LA-UR-21-29912)

Ultrafast Spectroscopy of Hybrid Quantum-plasmonic Nanoscale Optical Systems

Houtong Chen
20210845PRD1

Project Description

The goal of this project is to combine plasmonic structures, which control directional light flow at the nanoscale, with atomically thin two-dimensional quantum materials, which can provide new materials functionality, allowing us to enhance light-matter interactions with these hybrid nanostructures for a host of potential applications. This directly impacts national initiatives in quantum information science, which will underpin a host of future applications (e.g., quantum computing, secure communications, etc.). It will also address Department of Energy (DOE)/National Nuclear Security Administration (NNSA) priorities in next generation quantum systems, quantum materials, and ultrafast science. Finally, we anticipate potential connections to several DOE/NNSA missions, including the development of new materials and approaches for global security as well as novel approaches to quantum transduction that could impact optical communications.

Emergent Phenomena in Magnetically Frustrated f-electron Quantum Materials

Priscila Rosa
20210912PRD2

Project Description

Magnetically frustrated quantum materials show great potential for future technologies, such as quantum computation or high-density memory storage, but identifying suitable materials with ideally frustrated magnetic interactions remains an outstanding challenge within this field. In this project, we aim at synthesizing and investigating quantum materials that minimize existing bottlenecks by specifically targeting magnetic properties of underexplored f-electron-based frustrated lattices with appropriate magnetic interactions. Two types of f-electron materials will be investigated in which quantum spin liquid ground states or spin textures are predicted to appear. Ultimately, this project will lead to predictive understanding of unusual magnetic states in the fully quantum regime as a function of chemical and electronic tunability.

Publications

Presentation Slides

Bordelon, M. M., C. P. M. Girod, S. M. Thomas, J. D. Thompson, E. D. Bauer and P. Rosa. Unusual antiferromagnetism and field-induced transitions in tetragonal CeLiBi2. Presented at *International Conference on Strongly Correlated Electron Systems*, Campinas, Brazil, 2021-09-27 - 2021-10-02. (LA-UR-21-28184)

Rosa, P., S. M. Thomas, C. P. M. Girod, J. D. Thompson and E. D. Bauer. Unusual magnetism and field-induced transitions in Cerium-based materials. Presented at *New directions in strong correlation physics: From strange metals to topological superconductivity*, Aspen, Colorado, United States, 2022-01-23 - 2022-01-28. (LA-UR-22-20362)

Programmable Waveguides of Spin-Polarized Current with "Twisted" Moire Crystals

Scott Crooker
20210913PRD2

Project Description

Two-dimensional (2D), atomically-thin materials are poised to revolutionize electronics and opto-electronics technologies. The most well-known example is graphene, discovered in 2004, which is a single atomic layer of carbon atoms: graphene exhibits remarkable electronic properties such as high electrical conductivity and also remarkable mechanical properties such as high strength. More recently, other 2D materials have been discovered that exhibit additional technologically useful properties, such as semiconducting behavior (which allows for light-emitting and light-detection capabilities) and also magnetism (which allows for information storage and processing). This project is focused on exploring a hybrid route towards achieving magnetic functionality in 2D semiconductors such as molybdenum diselenide (WSe2) to achieve electrically-controllable magnetism -- a longstanding goal in the broad field of semiconductor electronics, with immediate technological relevance in the areas of data storage and information processing (ie, computing).

Publications

Journal Articles

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

Presentation Slides

Choi, J. Twist-Angle Controls Interlayer Exciton Dynamics in Transition Metal Dichalcogenide (TMD) Bilayers. Presented at *Theme Meeting at Center for Nanophase Materials Sciences in Oak Ridge National Laboratory*, Oak Ridge, Tennessee, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-23522)

High-performance Photo-sensor/detector by Multiplexed Heterojunction of 2-Dimensional Epitaxial Layers/perovskites/plasmonic Nanoparticles

Aiping Chen
20210945PRD2

Project Description

Photodetectors play critical roles in various optoelectronic applications. The key challenges to the practical applications are the balance between the photoresponsivity, selectivity and stability apart from the cost. This project will develop a hybrid material platform based on the engineered design of 2-Dimensional (2D) epitaxial layers, perovskites and plasmonic nanoparticles for high performance tunable broadband photodetectors. Such hybrid structure is deemed to take the advantage of high carrier mobility of 2D layers and superior optical absorption coefficient of perovskite, and excellent localized surface plasmon resonance of perovskite nanoparticles (PNPs). The successful development of materials and devices would provide an alternative path towards the design of high-performance photodetectors with wider spectral selectivity for advanced communication, imaging, and sensing applications. At the end of this project, we expect to optimize the plasmonic nanoparticles size and distribution in a film matrix of semi-conducting oxides or halide perovskite to achieve enhanced ultraviolet (UV) phototector performance such as fast response time and high sensitivity with low cost for high performance tunable broadband photodetector applications.

Publications

Journal Articles

Kunwar, S. MoS_2 Nanoflake and ZnO Quantum Dot Blended Active Layers on AuPd Nanoparticles for UV Photodetectors. Submitted to *ACS Applied Nano Materials*. (LA-UR-22-20997)

Kunwar, S. Plasmonic Core–Shell–Satellites with Abundant Electromagnetic Hotspots for Highly Sensitive and Reproducible SERS Detection. Submitted to *International Journal of Molecular Sciences*. (LA-UR-22-20995)

Electrocatalysts for Entirely Platinum Group Metal-free Water Electrolyzer

Piotr Zelenay
20210953PRD3

Project Description

This project directly addresses the important national security challenge of producing "green" hydrogen using electricity from renewable sources and at a competitive cost. Production of hydrogen via water electrolysis in low temperature water electrolyzers (LTEs) is especially attractive thanks to the close to ambient operating conditions and fast startup/shutdown, enabling an effective use and storage of the intermittent electricity from renewable sources (solar, wind). Current LTEs suffer from two main drawbacks: the use of highly corrosive solutions and the need for expensive catalysts based on precious metals. Recent advancements in performance and stability of anion exchange membranes (AEM) have enabled a new alkaline membrane-based LTE technology capable of successfully competing with incumbent technologies. This project will focus on the development of high-performance and low-cost catalysts for the AEM LTEs utilizing electrocatalysts based on earth-abundant elements. It will enable the deployment a technology for "green" hydrogen generation, with the ultimate goal of facilitating the transition to new energy systems based on renewable sources and thus mitigating the effects of global warming.

In Operando Study of Resistive-switching Devices at Nanoscale

Aiping Chen
20210954PRD3

Project Description

Resistive-switching (RS) observed in a variety of transitional-metal oxides is of great research interest since it opens up enormous opportunities in next-generation integrated electronics such as nonvolatile memory, and neuromorphic computing devices etc. Recent advances have shown a new interface-type RS devices with lower operation current and more reliable switching repeatability could revolutionize data storage and neuromorphic computing. However, the mechanisms of such interface-type devices are not clearly understood, which hinders the design and application of the new interface-type devices for memory and neuromorphic computing. This work, if successful, will for the first time allow us to directly observe oxygen vacancies migrations process in-situ in memristors during operation at the nanoscale in electron microscopy. The physical principles discovered in this work will be critical to design memristor devices for next generation memory devices and neuromorphic computing. Developing advanced microelectronic devices underpins the Department of Energy-Basic Energy Science research interests in "Microelectronics" and "Beyond Moore".

Conformal Field Theories with the Bootstrap

Anna Hayes-Sterbenz
20180709PRD1

Project Description

The ultimate goal of this project is to help the development of new materials with properties suitable for applications in high-performance electrical circuits and quantum computing. This pursuit is extremely relevant for national security, for it holds the promise of significant technological and computational advances. Through the theoretical study of newly discovered critical theories with promising properties, the project aims to provide a solid framework for further theoretical developments, and to guide the experimental effort for the development of new materials.

Technical Outcomes

Both liquids and crystalline materials have first-order phase transitions. The phase transition lines terminate at critical points, like the point where water can be a solid, liquid, or gas. This project developed a universal approach to the physics of these critical points. The numerical conformal bootstrap provides a widely-applicable and robust method for their study. The team explained, for the first time, a host of experimental results pertaining to various types of phase transitions.

Publications

Journal Articles

Henriksson, J., S. R. Kousvos and A. Stergiou. Analytic and Numerical Bootstrap of CFTs with O(m) $\times$ O(n) Global Symmetry in 3D. Submitted to *SciPost Physics*. (LA-UR-20-23147)

*Henriksson, J. and A. Stergiou. Perturbative and nonperturbative studies of CFTs with MN global symmetry. 2021. *SciPost Physics*. **11** (1): 015. (LA-UR-21-20310 DOI: 10.21468/SciPostPhys.11.1.015)

*Kousvos, S. and A. Stergiou. Bootstrapping mixed correlators in three-dimensional cubic theories II. 2020. *SciPost*. **8** (6): 085. (LA-UR-19-30978 DOI: 10.21468/SciPostPhys.8.6.085)

*Lin, Y., D. Meltzer, S. Shao and A. Stergiou. Bounds on Triangle Anomalies in (3+1)d. 2020. *Physical Review D*. **101** (12): 125007. (LA-UR-19-30323 DOI: 10.1103/PhysRevD.101.125007)

*Manenti, A., A. Vichi and A. Stergiou. Implications of ANEC for SCFTs in four dimensions. 2020. *Journal of High Energy Physics*. **2020** (1): 93. (LA-UR-19-25902 DOI: 10.1007/JHEP01(2020)093)

Mottola, E., A. Sadofyev and A. Stergiou. Effective Field Theory and Axions in Weyl Semimetals. Submitted to *Physical Review Letters*. (LA-UR-21-20979)

Osborn, H. and A. Stergiou. Heavy Handed Quest for Fixed Points in Multiple Coupling Scalar Theories in the \xce\xb5 Expansion. Submitted to *Journal of High Energy Physics*. (LA-UR-20-27569)

*Stergiou, A. Bootstrapping MN and tetragonal CFTs in three dimensions. 2019. *SciPost Physics*. **7** (1): 010. (LA-UR-19-25903 DOI: 10.21468/SciPostPhys.7.1.010)

*Stergiou, A. and S. Kousvos. Bootstrapping mixed correlators in three-dimensional cubic theories. 2019. *SciPost Physics*. **6** (3): 035. (LA-UR-19-25906 DOI: 10.21468/SciPostPhys.6.3.035)

*Stergiou, A. and S. Rychkov. General properties of multiscalar RG Flows in d=4−\xce\xb5. 2019. *SciPost Physics*. **6** (1): 008. (LA-UR-19-25904 DOI: 10.21468/SciPostPhys.6.1.008)

Presentation Slides

Stergiou, A. Uncovering the Structure of the \xce\xb5 Expansion. Presented at *University of Crete HEP Seminars*, Heraklion, Greece, 2020-10-06 - 2020-10-06. (LA-UR-20-27835)

Stergiou, A. Conformal Bootstrap and Continuous Phase Transitions in 3D. Presented at *ERG 2020*, Kyoto, Japan, 2020-11-02 - 2020-11-06. (LA-UR-20-28986)

Stergiou, A. Conformal Bootstrap and Critical Phenomena. Presented at *LANL P/T Colloquium*, Los Alamos, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20104)

Stergiou, A. Strongly-coupled Physics Through a Conformal Field Theory Lens (IC project w20_strongcftlens). . (LA-UR-21-21777)

Exploration of New Topological States of Matter in Strongly Correlated Materials and in Ultra-high Magnetic Fields

Neil Harrison
20180713PRD2

Project Description

The use of the world-unique 100 Tesla (T) capability at the Los Alamos National High Magnetic Field Laboratory (NHMFL) and f-electron materials to search for novel topological phases will open up a new field of research on topology in strongly correlated matter. Topology is seen as a promising route for the development of new electronics and quantum computation, and it is therefore in the national interest to develop the highest quality materials. It is anticipated that several entirely new regimes of physics will emerge in very strong magnetic fields. This project will help establish Los Alamos as a world-leader in topology at extremely high magnetic field and in topological materials with strong electronic correlations.

Technical Outcomes

The project's measurements in strong magnetic fields enabled significant advances in our understanding of topological Kondo insulating materials . This puts Los Alamos in a stronger position for addressing the question as to whether Kondo insulators are also topological materials.

Publications

Journal Articles

*Boschini, F., D. Bugini, M. Zonno, M. Michiardi, R. P. Day, E. Razzoli, B. Zwartsenberg, M. Schneider, E. H. Da Silva Neto, S. Dal Conte, S. K. Kushwaha, R. J. Cava, S. Zhdanovich, A. K. Mills, G. Levy, E. Carpene, C. Dallera, C. Giannetti, D. J. Jones, G. Cerullo and A. Damascelli. Role of matrix elements in the time-resolved photoemission signal. 2020. *Physical Review B*. **22** (2): 23031. (LA-UR-18-30021 DOI: 10.1088/1367-2630/ab6eb1)

*Cai, S., J. Guo, V. A. Sidorov, Y. Zhou, H. Wang, G. Lin, X. Li, Y. Li, K. Yang, A. Li, Q. Wu, J. Hu, S. K. Kushwaha, R. J. Cava and L. Sun. Independence of topological surface state and bulk conductance in three-dimensional topological insulators. 2018. *npj Quantum Materials*. **3** (1): 62. (LA-UR-19-26035 DOI: 10.1038/s41535-018-0134-z)

*Cai, S., S. K. Kushwaha, J. Guo, V. A. Sidorov, C. Le, Y. Zhou, H. Wang, G. Lin, X. Li, Y. Li, K. Yang, A. Li, Q. Wu, J. Hu, R. J. Cava and L. Sun. Universal superconductivity phase diagram for pressurized tetradymite topological insulators. 2018. *Physical Review Materials*. **2** (11): 114203. (LA-UR-19-26036 DOI: 10.1103/PhysRevMaterials.2.114203)

*Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. F. S. Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Nature Communications*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

*Rosa, P., Y. Xu, M. Rahn, J. Souza, S. Kushwaha, L. Veiga, A. Bombardi, S. Thomas, M. Janoschek, E. Bauer, M. Chan, Z. Wang, J. Thompson, N. Harrison, P. Pagliuso, A. Bernevig and F. Ronning. Colossal magnetoresistance in a nonsymmorphic antiferromagnetic insulator. 2020. *npj Quantum Materials*. **5** (1): 52. (LA-UR-20-20098 DOI: 10.1038/s41535-020-00256-8)

Presentation Slides

Kushwaha, S. K. Development and study of the novel topological quantum materials. Presented at *Invited Colloquium*, Kalamazoo, Michigan, United States, 2020-03-16 - 2020-03-17. (LA-UR-20-22457)

Kushwaha, S. K. Development and study of novel topological materials. Presented at *Interview presentation*, Houston, Texas, United States, 2020-07-29 - 2020-07-29. (LA-UR-20-25748)

Kushwaha, S. K., M. K. Chan, N. Harrison, P. Ferrari Silveira Rosa, S. M. Thomas, E. D. Bauer, F. Ronning, J. Park and J. D. Thompson. Magnetic field induced Fermi liquid in a candidate topological Kondo insulator. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22244)

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, E. D. Bauer, J. D. Thompson, J. Zhu, C. Cao, F. Ronning and N. Harrison. Insulator/metal transition in a Topological Kondo Insulator at 60 T. Presented at *NSF meeting*, Tallahassee, Florida, United States, 2018-11-14 - 2018-11-14. (LA-UR-18-30652)

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, E. D. Bauer, J. D. Thompson, J. Zhu, F. Ronning, N. Harrison and C. Chao. Transport and magnetic properties of correlated Ce3Bi4Pd3 at high magnetic fields. Presented at *APS March Meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-08. (LA-UR-19-23573)

Kushwaha, S. K., M. K. Chan, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa, N. Harrison and J. Park. Metallization and Fermi-liquid state in a Kondo-insulator in high magnetic fields. Presented at *Dynamic Quantum Matter and Materials*, Jacksonville, Florida, United States, 2020-12-14 - 2020-12-16. (LA-UR-20-30245)

Posters

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning and N. Harrison. Field induced metallic state in Ce3Bi4Pd3 Correlated Kondo material. Presented at *CNLS 39th Annual Conference - Strongly Correlated Quantum Materials*, Santa Fe, New Mexico, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-23792)

Development of an Innovative Mechanical Testing System and Techniques for Characterizing Irradiated Advanced Cladding Concepts and Novel Materials

Jonathan Gigax
20180744PRD3

Project Description

The goal of this project is to develop a novel in situ mechanical testing devices to perform analysis on specimen volumes on the microscale and approaching the macroscale. The device (commercially unavailable) will integrate high temperature and high strain rate capabilities to probe the mechanical response under extreme conditions. Macroscale mechanical testing of neutron irradiated materials has been used extensively to understand mechanical property (tensile, ductility, creep, hardness) changes after irradiation. Such testing is critical to the continued safe operation of the nuclear reactor as dramatic changes in mechanical properties (i.e. embrittlement) may result in fuel cladding failure and undesired radioactivity release. Thus, the development of mechanical testing techniques on the mesoscale enables one to obtain data from small volumes (e.g. produced by ion irradiation) and samples with larger (bulk) volumes irradiated by neutrons to obtain data that is essential to further validate mechanical testing of ion irradiated alloys and advance materials development for next generation nuclear reactors such as those being developed in DOE's Nuclear Energy Programs.

Technical Outcomes

The first outcome of this project was centered around the development of techniques and equipment necessary to perform mechanical testing on the mesoscale. Femtosecond laser ablation techniques combined with a quasi-static test system, and a high strain rate system were developed to study the mechanical behaviors of materials on this length scale. The second outcome was the successful deployment of these techniques to nuclear reactor structural materials and novel material systems.

Publications

Journal Articles

Gigax, J. G., A. J. Torrez, Q. Mcculloch, H. Kim, S. A. Maloy and N. Li. Sizing up mechanical testing: Comparison of microscale and mesoscale mechanical testing techniques on a FeCrAl welded tube. Submitted to *Journal of Materials Research*. (LA-UR-19-32551)

*Gigax, J. G., H. Vo, Q. McCulloch, M. Chancey, Y. Wang, S. A. Maloy, N. Li and P. Hosemann. Micropillar compression response of femtosecond laser-cut single crystal Cu and proton irradiated Cu. 2019. *Scripta Materialia*. **170**: 145-149. (LA-UR-19-21957 DOI: 10.1016/j.scriptamat.2019.05.004)

*Gigax, J. G., J. K. Baldwin, C. J. Sheehan, S. A. Maloy and N. Li. Microscale shear specimens for evaluating the shear deformation in single-crystal and nanocrystalline Cu and at Cu–Si interfaces. 2019. *Journal of Materials Research*. **34** (9): 1574-1583. (LA-UR-19-21222 DOI: 10.1557/jmr.2019.104)

Gigax, J. G., O. El Atwani, Q. Mcculloch, B. Aytuna, M. Efe, S. J. Fensin, S. A. Maloy and N. Li. Micro- and mesoscale mechanical properties of an ultra-fine grained FeCrMnNi high entropy alloy produced by large strain machining. Submitted to *Scripta Materialia*. (LA-UR-19-29789)

Mcculloch, Q., J. G. Gigax and P. Hosemann. Femtosecond laser ablation for mesoscale specimen evaluation. Submitted to *JOM*. (LA-UR-19-27649)

Reports

Gigax, J. G., H. Kim, M. R. Chancey, Y. Wang and N. Li. Heavy Ion Irradiation Characterization of C26M. Unpublished report. (LA-UR-20-28209)

Gigax, J. G. and N. Li. Microstructural and Nanomechanical Characterization of FeCrAl Pressure Resistance Welds. Unpublished report. (LA-UR-20-27950)

Presentation Slides

Gigax, J. G., N. Li, Q. Mcculloch, H. Kim, M. R. Chancey, Y. Wang, C. R. Lear, S. A. Maloy and P. Hosemann. Novel Small Scale Mechanical Testing Techniques for Nuclear Materials. Presented at *TMS 2021 Spring (online)*, Orlando, Florida, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-21722)

Gigax, J. G., N. Li and S. A. Maloy. Nb Weld Overview. . (LA-UR-20-26513)

Gigax, J. G., O. El Atwani, M. R. Chancey, J. K. S. Baldwin and S. A. Maloy. Nanomechanical Properties of Pristine and Heavy Ion Irradiation Nanocrystalline Tungsten. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-28. (LA-UR-20-21593)

Gigax, J. G., Q. Mcculloch, S. A. Maloy, P. Hosemann and N. Li. Femtosecond laser ablation techniques for mesoscale specimen analysis. Presented at *University of California Berkeley Mechanics Workshop*, Berkeley, California, United States, 2020-03-02 - 2020-03-03. (LA-UR-20-21927)

Gigax, J. G., S. A. Maloy and N. Li. Novel micro- and mesoscale techniques for mechanical property characterization and their applications. . (LA-UR-21-20723)

Posters

Gigax, J. G., N. Li and S. A. Maloy. Micro- and Mesoscale Mechanical Methods for Material Extremes. Presented at *Materials Capability Review 2020*, Los Alamos, New Mexico, United States, 2020-04-30 - 2020-04-30. (LA-UR-20-22896)

Gigax, J. G., O. El Atwani, Q. Mcculloch, B. Aytuna, M. Efe, S. J. Fensin, S. A. Maloy and N. Li. Micro- and mesoscale mechanical properties of an ultra-fine grained CrFeMnNi high entropy alloy produced by large strain machining. Presented at *TMS 202*, San Diego, California, United States, 2020-02-23 - 2020-02-28. (LA-UR-20-21399)

Other

Gigax, J. G., T. Ajantiwalay and S. A. Maloy. Compression of mesoscale pillars in unirradiated HT9 and HT9 irradiated with protons up to 0.1 dpa. Audio/Visual. (LA-UR-20-28091)

Ferromagnetism and Spin Fluctuations in the Atomically-Thin Limit

Scott Crooker
20180747PRD3

Project Description

Two-dimensional (2D), atomically-thin materials are poised to revolutionize electronics and opto-electronics technologies. The most well-known example is graphene, discovered in 2004, which is a single atomic layer of carbon atoms: graphene exhibits remarkable electronic properties such as high electrical conductivity and also remarkable mechanical properties such as high strength. More recently, other 2D materials have been discovered that exhibit additional technologically useful properties, such as semiconducting behavior (which allows for light-emitting and light-detection capabilities) and also magnetism (which allows for information storage and processing). This project is focused on exploring an entirely new route towards achieving magnetism in a new class of 2D materials based on the semiconductor gallium selenide (GaSe). Recent theory indicates that magnetic behavior can be induced in GaSe by electrical means. Electrically-controllable magnetism is a longstanding 'holy grail' in the broad field of semiconductor electronics, with immediate technological relevance in the areas of data storage and information processing (ie, computing).

Technical Outcomes

Using optical spectroscopy in some of the world's largest magnetic fields, this project demonstrated that two-dimensional semiconductors can indeed, as long predicted, exhibit a spontaneous transition to a ferromagnetic state. Separately, we systematically measured the intrinsic dynamical properties of electrons in these materials.

Publications

Journal Articles

Crooker, S. A., M. Goryca, J. Li, S. Tongay, K. Yumigeta and H. Li. Carrier-density-dependent valley relaxation in a monolayer semiconductor and the role of substrate-induced disorder. Submitted to *Physical Review Applied*. (LA-UR-21-20744)

*Goryca, M., J. Li, A. V. Stier, T. Taniguchi, K. Watanabe, E. Courtade, S. Shree, C. Robert, B. Urbaszek, X. Marie and S. A. Crooker. Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields. 2019. *Nature Communications*. **10** (1): 4172. (LA-UR-19-23579 DOI: 10.1038/s41467-019-12180-y)

*Goryca, M., X. Zhang, J. Li, A. L. Balk, J. D. Watts, C. Leighton, C. Nisoli, P. Schiffer and S. A. Crooker. Field-Induced Magnetic Monopole Plasma in Artificial Spin Ice. 2021. *Physical Review X*. **11** (1): 011042. (LA-UR-20-24139 DOI: 10.1103/PhysRevX.11.011042)

*Li, J., S. A. Crooker, M. M. Goryca, A. V. Stier, N. Wilson and X. Xu. Spontaneous Valley Polarization of Interacting Carriers in a Monolayer Semiconductor. 2020. *Physical Review Letters*. **125** (14): 147602. (LA-UR-20-25746 DOI: 10.1103/PhysRevLett.125.147602)

Posters

Li, J. and J. Zhu. Probing Quantum Hall and Quantum Valley Hall Effect in Bilayer Graphene Nanostructures. Presented at *The 46th Conference on the Physics and Chemistry of Surfaces and Interfaces (PCSI-46)*, Santa Fe, Minnesota, United States, 2019-01-13 - 2019-01-17. (LA-UR-19-20395)

In Situ Mesoscale Response under Combined Pressure-Shear Dynamic Loading

Cynthia Bolme
20190639PRD2

Project Description

A combined experiment and theory approach will be developed to perform in situ measurements of materials under pressure-shear shock loading. This work will result in better understanding of the mesoscale material deformation mechanisms and a computational model for simulating the material response. This work directly addresses the national security challenges related to the dynamic behavior of materials. The ability to understand and simulate pressure-shear shock conditions in low symmetry materials will be immediately useful to the mission areas of Dynamic Mesoscale Materials Science and to Stockpile Stewardship.

Technical Outcomes

The inclined impact experiments developed during this project will enable the generation and characterization of shearing deformation, which when applied to High Energy(HE) materials 1) enable the determination of crucial elastic constants, and 2) enable direct measurement of the shear strength under combined shock and shear. The computational tools developed are anticipated to play a crucial role for predicting the response of HE to sub- and weak-shock mechanical hazards, where crystal mechanics influences temperature localization.

Publications

Journal Articles

Zuanetti, B., D. J. Luscher, C. A. Bolme and K. J. Ramos. Unraveling the Implications of Finite Specimen Size on the Interpretation of Dynamic Experiments for Polycrystalline Aluminum through Direct Numerical Simulations. 2021. *International Journal of Plasticity*. 103080. (LA-UR-21-23050 DOI: 10.1016/j.ijplas.2021.103080)

*Zuanetti, B., D. J. Luscher, K. J. Ramos, C. A. Bolme and V. Prakash. Dynamic flow stress of pure polycrystalline aluminum: Pressure-shear plate impact experiments and extension of dislocation-based modeling to large strains. 2021. *Journal of the Mechanics and Physics of Solids*. **146**: 104185. (LA-UR-20-23354 DOI: 10.1016/j.jmps.2020.104185)

Posters

Zuanetti, B., C. A. Bolme, K. J. Ramos and D. J. Luscher. Investigation of the Mesoscale Response of Anisotropic Crystals under Combined Pressure-Shear Dynamic Loading. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27842)

Ex Machina Hamiltonians for Next-Generation Molecular Simulations

Galen Craven
20190642PRD3

Project Description

The project will apply advanced computer simulation methods to examine the molecular mechanisms underlying electrical and thermal conduction processes in emerging energy nanotechnologies with direct applications to sustainable energy initiatives. The two specific applications to be explored are electronic conduction in molecular nanodevices that operate at the human-machine interface and heat conduction in complex molecular devices. This proposal will advance the current understanding of molecular-level functionality in several energy nanotechnologies and could significantly impact DOE missions related to energy independence.

Technical Outcomes

The work in this project led to development of a machine learning method to determine structural, thermodynamic, and transport properties of condensed-phase systems with increased predictive accuracy in comparison with traditional theoretical methods. Variants of the machine learning methods from this project are currently being performed in projects which focus on the use of data-driven approaches to determine properties of nuclear fuels, for example, thermal and electrical conductivity.

Publications

Journal Articles

*Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. 2020. *The Journal of Chemical Physics*. **153** (10): 104502. (LA-UR-19-31421 DOI: 10.1063/5.0017894)

*Craven, G. T., N. Lubbers, K. Barros and S. Tretiak. Determination of Structural Correlation Functions. 2020. *The Journal of Physical Chemistry Letters*. **11** (11): 4372-4378. (LA-UR-19-32446 DOI: 10.1021/acs.jpclett.0c00627)

Reports

Craven, G. T. Analytical solutions of the Arrhenius-Semenov problem for constant volume burn. Unpublished report. (LA-UR-21-31229)

Presentation Slides

Craven, G. T. Data-Driven Determination of Correlation Functions. . (LA-UR-20-24825)

Craven, G. T. Machine learning approaches for thermodynamic and transport properties of fluids and materials. Presented at *Los Alamos - Arizona Days Conference 2021*, Los Alamos, New Mexico, United States, 2021-05-17 - 2021-05-18. (LA-UR-21-24657)

Other

Craven, G. T. Dataset and programs to calculate properties of a Lennard-Jones fluid. Dataset. (LA-UR-20-24204)

Exploration of Colossal Thermoelectric Power in 4-fundamental (4f) and 5f Topological Magnets

Filip Ronning
20190654PRD4

Project Description

This research project is well aligned with the Laboratory agenda on quantum information science. Topological materials are widely believed to provide a route to harnessing new functionality in quantum materials in the future. This research is designed to understand the origin of large topological effects in strongly correlated magnetic metals, which are particularly strong in actinide-based materials. The Berry curvature of a wavefunction creates an anomalous velocity, which produces large transverse voltages in topological materials. The large transverse voltage response has potential interest for spintronic applications, as well as developing fundamentally new states of matter. Here we will study how this large response varies as a function of alloying various actinide materials. This research will help elucidate the origin of large responses in materials, and hopefully demonstrate how to control their effects.

Technical Outcomes

Uranium contains both strong spin-orbit coupling and strong electronic correlations. This combination, plus a kagome lattice structure, leads to an enormous number of topological features in the ferromagnetic metal, "UCo0.8Ru0.2Al." The result is a new record for the colossal anomalous Peltier coefficient, which reflects a material's ability to convert heat to charge.

Publications

Journal Articles

*Asaba, T., S. M. Thomas, M. Curtis, J. D. Thompson, E. D. Bauer and F. Ronning. Anomalous Hall effect in the kagome ferrimagnet. 2020. *Physical Review B*. **101** (17): 174415. (LA-UR-20-20100 DOI: 10.1103/PhysRevB.101.174415)

Asaba, T., V. Ivanov, S. M. Thomas, S. Savrasov, J. D. Thompson, E. D. Bauer and F. Ronning. Colossal anomalous Nernst effect in a correlated noncentrosymmetric kagome ferromagnet. Submitted to *Science Advances*. (LA-UR-21-22548)

Hamann, D. M., S. P. Rudin, F. Ronning, T. Asaba, D. L. M. Cordova, P. Lu and D. C. Johnson. Emergent Structures and Properties in Interface Stabilized 2D-Layers. Submitted to *Science*. (LA-UR-19-31418)

Ronning, F., S. Lee, S. Seo, K. E. Avers, S. M. Thomas, R. Movshovich, J. D. Thompson, P. Rosa, E. D. Bauer and T. Asaba. Physical properties of quasi-one-dimensional YbFe5P3. Submitted to *Physical Review B*. (LA-UR-21-28341)

Presentation Slides

Asaba, T., V. Ivanov, S. M. Thomas, S. Savrasov, J. D. Thompson, E. D. Bauer and F. Ronning. Colossal anomalous Nernst effect in a correlated noncentrosymmetric kagome ferromagnet. Presented at *APS march meeting 2021 (online)*, Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-21064)

Electrically Driven Optoelectronic Plasmonic Nanodevice in Carbon Nanotubes

Andrew Jones
20200757PRD3

Project Description

Photonic systems lie at the heart of almost all modern technologies. They make high speed internet possible and can be found inside of your computers and television sets. This project aims toward developing a new class of ultra-compact and efficient infrared light emitters by exploiting a novel phenomenon called plasmonic, which involves the coupling between light and electrons with materials. The photonic devices less than 1 nanometer thick can be fabricated by using single nanostructures, called nanotubes, as building blocks for information transmission and light emission. These building blocks can also be integrated into existing silicon (Si) based electronic and photonic integrated circuits.

Technical Outcomes

This project was successful in achieving its preliminary goal of developing Los Alamos' capability to characterize the magnitude and spatial distribution of optical near-fields surrounding individual nanostructures in the mid-infrared (IR) spectral range. In addition to verifying the capability to measure one dimensional nanostructures, the project also characterized optical signals associated with two dimensional graphene sheets and grain boundaries. This observation opens the door for characterization of similar two dimensional nanophotonic devices.

Publications

Journal Articles

Wang, S., S. Yoo, S. Zhao, W. Zhao, S. Kahn, D. Cui, F. Wu, L. Jiang, I. B. Utama, H. Li, S. Li, A. Zibrov, E. Regan, D. Wang, Z. Zhang, K. Watanabe, T. Taniguchi, C. Zhou and F. Wang. Gate-tunable plasmons in mixed-dimensional van der Waals heterostructures. Submitted to *Nature Communications*. (LA-UR-21-28059)

Unconventional Topological Excitations in Correlated Materials

Nikolai Sinitsyn
20210809PRD1

Project Description

Novel atomically thin materials have unusual properties that are of interest to quantum information processing. This project will study these properties and provide estimates for feasibility of quantum information devices based on such materials.

Technical Outcomes

During the brief period of funding, about two months, the team prepared an article on simulations of Mott insulator on a quantum computer.

Publications

Journal Articles

Rodriguez-Vega, M. A., A. Baydin, F. G. G. Baydin, A. K. Okazaki, F. Tay, T. Noe II, I. Katayama, J. Takeda, H. Nojiri, P. H. O. Rappl, E. Abramof, G. A. Fiete and J. Kono. Magnetic Control of Soft Chiral Phonons in PbTe. Submitted to *Physical Review Letters*. (LA-UR-21-26398)

Rodriguez-Vega, M. A., D. Lujan, J. Choe, Z. Ye, A. Leonardo, T. N. Nunley, L. Chang, S. Lee, J. Yan, G. A. Fiete, R. He and X. Li. Magnons and magnetic fluctuations in atomically thin layers of MnBi2Te4. Submitted to *Nature Physics*. (LA-UR-21-26747)

Rodriguez-Vega, M. A., I. A. Assi, J. P. F. LeBlanc, H. Bahlouli and M. Vogl. Floquet engineering and non-equilibrium topological maps in twisted trilayer graphene. Submitted to *Physical Review B*. (LA-UR-21-25887)

Rodriguez-Vega, M. A., Z. Lin, A. Leonardo, A. Ernst, M. G. Vergniory and G. A. Fiete. Light-driven topological and magnetic phase transitions in thin-layer antiferromagnets. Submitted to *Physical Review X*. (LA-UR-21-27491)

Rust, Dust, and a Passive Future - Resilient Actinide Materials (U)

Samantha Lawrence
20200481MFR

Project Description

Despite years of research, unanswered fundamental questions persist surrounding the causes of uranium corrosion in hydrogen-containing environments. This project aims to understand the chemical reactions that take place at uranium metal surfaces that ultimately dictate corrosion rates. This will be accomplished by studying, for the first time, complimentary solution and gas-solid chemical reactions that occur under hydrogen-containing environments with uranium. The data obtained from this work will inform physics and chemistry-based models of uranium corrosion, which will ultimately enhance our predictive capability.

Publications

Presentation Slides

Lawrence, S. K. Studying Hydrogen-Metal Interactions at the Lujan Center. Presented at *Informal team meeting*, Online, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21879)

Lawrence, S. K. and D. T. Carver. In-situ hydriding of depleted uranium: A search for preferential nucleation sites. Presented at *NSLS-II & CFN Joint Users' Meeting*, Virtual, New York, United States, 2021-05-17 - 2021-05-20. (LA-UR-21-24890)

Solution fabricated solid-state X-ray imager

Wanyi Nie
20210533MFR

Project Description

X-ray imaging is a non-destructive tool that is widely used in advanced accelerators facility, nuclear material manufacturing and other material science applications. It requires highly sensitive detectors to image the X-ray signal. Semiconductor based X-ray imager that directly converts X-ray photon to electrical signal provides the best conversion efficiency among other technologies in ideal case. However, the current state-of-the-art technology uses amorphous selenium as X-ray absorber that suffers from poor charge extraction efficiency and high fabrication costs that undermines their wide use. We propose to fill the gap with demonstrating new semiconductor-based X-ray imager. Here, we will investigate lead-halide perovskite semiconductor, a solution processable material, for high resolution X-ray imager applications. Leveraging our previous breakthrough in high efficiency perovskite X-ray detector demonstration, we expect to build large scale imagers with high performances. The successful demonstration will provide new route for cost-effective X-ray imager fabrication with high sensitivity and spatial resolutions

Publications

Journal Articles

*Kobbekaduwa, K., S. Shrestha, P. Adhikari, E. Liu, L. Coleman, J. Zhang, Y. Shi, Y. Zhou, Y. Bekenstein, F. Yan, A. M. Rao, H. Tsai, M. C. Beard, W. Nie and J. Gao. In-situ observation of trapped carriers in organic metal halide perovskite films with ultra-fast temporal and ultra-high energetic resolutions. 2021. *Nature Communications*. **12** (1): 1636. (LA-UR-20-27180 DOI: 10.1038/s41467-021-21946-2)

Pan, L., S. Shrestha, N. Taylor, W. Nie and L. R. Cao. Determination of X-ray detection limit and applications in perovskite X-ray detectors. 2021. *Nature Communications*. **12** (1): 5258. (LA-UR-21-28788 DOI: 10.1038/s41467-021-25648-7)

Shrestha, S., X. Li, H. Tsai, C. Hou, H. Huang, D. Ghosh, J. Shyue, L. Wang, S. Tretiak, X. Ma and W. Nie. Long carrier diffusion length in two-dimensional lead halide perovskite single crystals. Submitted to *CHEM*. (LA-UR-21-29516)

Tsai, H., H. Huang, J. D. Watt, C. Hou, J. Strzalka, J. Shyue, L. Wang and W. Nie. Cesium lead halide perovskite nanocrystals assembled in metal-organic frameworks for stable blue light emitting diodes. Submitted to *Advanced Materials*. (LA-UR-21-30401)

Tsai, H., S. Shrestha, L. Pan, H. Huang, J. Strzalka, D. J. Williams, L. Wang, R. Cao and W. Nie. Quasi-2D perovskite crystalline layers for printable direct conversion X-ray imaging. Submitted to *Advanced Materials*. (LA-UR-21-29520)

Presentation Slides

Nie, W. Low-dimensional Metal Halide Hybrid Perovskite Semiconductors for Light Emitting Devices. Presented at *Material Research Society, spring 2021*, Web meeting, New Mexico, United States, 2021-04-21 - 2021-04-27. (LA-UR-21-23773)

Nie, W. Emerging solution processible perovskite semiconductors for solid-state detectors. Presented at *3rd International Conferences on Nuclear Photonics, web meeting*, Online, Japan, 2021-06-07 - 2021-06-11. (LA-UR-21-25365)

Nie, W. Halide perovskite based opto-electronics: light emitting diodes and solid-state detectors. . (LA-UR-21-29270)

Modern Radiation Case Material for an Agile Complex

Kendall Hollis
20210536MFR

Project Description

Evaluating new materials and technologies that were not available during cold war nuclear weapon development could provide future weapon systems with radiation cases that are lower in cost, lower in worker health risk and lower in environmental impact while delivering certified robust performance in a development and manufacturing time efficient manner. Using the latest available tools in physics modeling and material fabrication, this investigation will evaluate materials and recommend the most promising ones to be considered as alternatives to current materials and manufacturing technologies.

High -Performance/-Precision/-Z (HPPZ) Scintillator Grids via Advanced Electrochemistry

Enkeleda Dervishi-Whetham
20210572MFR

Project Description

Imaging is a critical element of measurements involving x-rays and other forms of non-visible probes to provide snapshots of dynamic events. Scintillators are used to convert the signal received to an electronic or visible signature. For spatial resolution, individual scintillators must be in a separated array, providing fine detail in closely spaced pixels with no cross-communication. Small (millimeter) scintillation crystals need to be spaced by micrometers, separated by very dense and high-atomic number materials. This is difficult or impossible to achieve through traditional techniques, and therefore is a major limitation of high-precision dynamic imaging. New pulse- and pulse-reverse electrochemical methods provide a pathway to solve this problem, and this project will demonstrate the application of these new methods to create high-precision micron-scale grids of gold and rhenium that can be scaled to any needed dimension. The development of practical methods to achieve high-precision large format future scintillators will have a major impact on advanced dynamic imaging needs. The end products will be useful to current mission needs and provide foundational research for other materials and applications. Further, the development of the technique itself will provide methods for processing dense, difficult to process materials, opening up other possible applications.

Publications

Journal Articles

Dervishi-Whetham, E. and D. E. Hooks. Mechanical and tribological properties of anodic Al coatings as a function of anodizing conditions. Submitted to *Surface & Coatings Technology*. (LA-UR-21-32123)

Presentation Slides

Dervishi-Whetham, E. High -Performance/-Precision/-Z(HPPZ) Scintillator Grids via Advanced Electrochemistry Phase

I – Project # 20210572MFR- Mid year review. . (LA-UR-21-22404)

Modernizing Detonator Production and Inspection: Robotics meets Additive and Digital Manufacturing

Alexandria Marchi
20200437MFR

Project Description

This project aims to create a new paradigm for detonator design and manufacturing towards enhancing the technological readiness of our detonator production agency. The Laboratory has the mission to supply detonators to a wide range of explosive operations and missions both at Los Alamos and across the Nuclear Security Enterprise, ranging from research and development tests, to Hydros and proton radiography (pRAD) shots at Los Alamos, to SubCritical Shots at Nevada National Security Site (NNSS) and across the Complex. Through advanced manufacturing investments targeting detonator production, advanced detonator design concepts may be considered, designed, manufactured, and tested all at Los Alamos in a fraction of the time and expense currently required because of extended manufacturing capabilities between industry and multiple complexes. Advanced manufacturing processes are critical for efficient, flexible, and agile responsiveness across the nuclear weapons complex.

Technical Outcomes

Limitations of the traditional detonator manufacturing scheme drove the following technical goals/achievements: 1) the team designed a robot-based work cell to coordinate manufacturing, inspection, and assembly on a single platform, 2) optical inspection techniques were analyzed to replace and/or supplement coordinate-measuring machines (CMMs) and manual inspection, 3) detonator headers were printed via additive manufacturing from materials with sufficient resolution and irradiation stability, 4) the team tested an improved an assembly scheme only feasible from the methods developed.

Integrating Additive Manufacturing and Investment Casting for Complex Metal Architectures with Predictable Mechanics (U)

Matthew Lee
20200450MFR

Project Description

3-Dimensional (3-D) printed metals can potentially advance several key Department of Energy (DOE)/ National Nuclear Security Administration (NNSA) missions related to stockpile modernization and retrofit, enhanced surveillance, and space applications. However, the properties of printed metals can be difficult to predict and reproduce, and historically this has impeded the adaptation of 3-D printing technology in many applications pertinent to the DOE. This project aims to bridge the gap between old and new technologies by hybridizing 3-D printing with traditional investment casting. The goal is to create new manufacturing techniques wherein 3-D printing is used to create hollow ceramic molds into which metals can be directly cast; this will achieve both the free-form design of printed objects with the predictable and reliable properties of cast metals. We expect to develop a simple collection of manufacturing techniques that can be used to create any castable metal with nearly any 3-D geometry. In turn, this will open up new applications in nuclear weapon design, satellites and other aerospace technologies, and national security, wherein high-precision metal components with exotic design are currently needed to enhance the performance of engineered systems.

Technical Outcomes

This project was successful in developing a new class of water-soluble ceramic coatings for investment casting. Know as Wash-Away Fine-Feature Low-Effort (WAFFLE) coatings, the team had success in formulating a number of WAFFLEs based entirely on non-toxic and commercial off-the-shelf constituents. WAFFLE coatings were proven to withstand temperatures exceeding 1000 Celsius without loss of solubility after the metal casting was complete. Finally, the team performed crucial initial studies on WAFFLE for depleted uranium casting.

Publications

Presentation Slides

Lee, M. N., K. J. Cluff, J. C. Cooley, R. R. Collino, M. E. Sherrill and R. S. Baty. WAFFLE – An Advanced Manufacturing Concept. Presented at *Weapons Capability Review*, Los Alamos, New Mexico, United States, 2021-08-25 - 2021-08-25. (LA-CP-21-20690)

Special Carbide for Weapon Applications (U)

David Jablonski
20200461MFR

Project Description

The novel use of a ceramic in weapons has become of increasing interest to the weapons community. This application of the ceramic has very attractive characteristics for use in the nuclear stockpile. The material is challenging to fabricate, but in recent years Los Alamos has made significant advances in the necessary technologies. The objective of this project is to integrate these technologies and demonstrate the fabrication of the material in a form that could be used in a weapon.

Technical Outcomes

The project had three objectives: fabricate the ceramic, execute explosively driven experiments with the ceramic, and model the behavior of the ceramic with our physics simulation tools. The team began with small material samples and progressed to full-sized parts. The capstone experiment fired in mid-September delivered excellent diagnostic data which the team continues to digest and interpret. A solid foundation has been laid to use the ceramic in weapon projects in FY22 and future years.

Publications

Reports

C. Triola, C. L., C. C. Joggerst, C. Chen, T. J. Foley and D. F. Jablonski. Simulations of Sweeping Wave Propagation in a Boron Carbide Plate. Unpublished report. (LA-UR-20-29040)

The Use of Additive Manufacturing of High Explosives and its Application to Weapon Safety (U)

Von Whitley
20200463MFR

Project Description

This project will investigate the possibility of using additive manufacturing (AM) of high explosives (HE) to produce a structured explosive whose detonation property can be turned on or off depending on the system configuration. In a single component configuration, the structure of the explosive will prevent detonation propagation under any external impulse (unintentional or accidental use). With the addition of a secondary liquid component, the binary mixture will allow a detonation to occur. The secondary component can be either reactive (liquid explosive) or inert (water) depending on performance and safety needs of the application.

Technical Outcomes

This project successfully demonstrated detonation control. Experiments clearly indicated that we could turn the detonation of an additively manufactured explosive on and off with the addition of a secondary component. The secondary component needed to switch the detonation to the 'ON' state could either be an explosive or an inert like water. Computation modeling was used to predict this switchability and experiments verified the accuracy of the computation.

Publications

Presentation Slides

J. Coffelt, C. A. Los Alamos Summer Project 2020. . (LA-UR-20-27795)

Mueller, A. H., A. M. Schmalzer, V. H. Whitley, P. R. Bowden and B. C. Tappan. Applications of HE additive manufacturing at LANL. Presented at *JOWOG AM 2020*, livermore, California, United States, 2020-01-27 - 2020-01-30. (LA-CP-20-20039)

Prompt, Photogated Negative Hydrogen Source

Rodney Mccrady
20200468MFR

Project Description

Los Alamos Neutron Science Center (LANSCE) is a particle accelerator at Los Alamos that is used for a variety of basic science and mission-driven experiments. These measurements require a negative hydrogen (H-) ion beam. The current source for this beam uses a plasma as well as a large amount of highly reactive cesium. This makes it very difficult to operate and understand, and often results in reduced performance or even reduced user time as a result. This project will use light, atomic hydrogen, and solid state materials similar to those used in solar cells and sensors to produce the first demonstration of a light controlled H- beam. The individual components required are all heavily used by various industries, largely computing related. This means that the technology for the individual components is extremely well developed. This will make it easier to make a well understood, adaptable source. This experiment will be the first ever demonstration and will give insights on how to scale and optimize the process for a future prototype that could be tested at Los Alamos and could potentially replace the currently used source if successful.

Technical Outcomes

The project successfully designed an experiment to measure the current and beam properties of negative Hydrogen (H-) produced via an excitation source (electron gun or laser) interacting with an engineered semconductor. H- was not produced, which was highly unexpected, as all models published to date suggest that the conditions should have been very efficient at producing H-. Two mechanisms not considered in models have been identified: adsorption and insufficient electron supply, these mechanisms are currently being probed.

Publications

Journal Articles

Alexander, A. M., M. Gaowei, S. Mistry, J. Walsh, F. Liu, K. Evans-Lutterdot, E. Stavitski, V. Pavlenko, K. Attenkofer, J. M. Smedley and N. A. Moody. Robust method for broadband efficiency enhancement of electron photocathodes using optical interferences. Submitted to *Applied Physics Letters*. (LA-UR-21-22492)

Presentation Slides

Banerjee, S. Theory and modeling of quantum mechanical transport for electron and negative-ion sources. Presented at *2021 Virtual theoretical Division Lightning Talks*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-28017)

Understanding Homogenization Kinetics of As-Cast Plutonium Alloys to Improve Manufacturing of Weapons Components (U)

Jeremy Mitchell
20200474MFR

Project Description

One of the most time-consuming steps of plutonium (Pu) manufacturing is the post-casting thermal treatment needed to homogenize and stabilize as-cast Pu-Ga (Plutonium-Gallium) alloys. Through careful experiments on a series of well-characterized samples, we will replicate manufacturing processes with in-situ diagnostics to assess the optimal heat treatment for these alloys. This science-based approach to weapons manufacturing will be useful in optimizing the homogenization process and has the potential for time reduction in one step of the plutonium manufacturing process.

Technical Outcomes

This project was highly successful in addressing the primary goals and objectives. In particular, the team assembled a comprehensive database and understanding of homogenization kinetics and resulting phase stability of an as-cast Pu-Ga (Plutonium-Gallium) alloy. This work is influencing the manufacturing community as evidenced by carry-on funding through Plutonium Modernization. This work allowed a better understanding of the phase stability of R&D castings, particularly those made for Office of Experimental Science.

In-Situ Ultrasound Grain Refinement in Electron Beam Additive Manufacturing for Improvement of High Strain-Rate Properties (U)

Cristian Pantea
20200500MFR

Project Description

Electron Beam Additive Manufacturing (EBAM) has potential applications with respect to the stewardship of the nation's nuclear weapons stockpile. The resulting metal structure of the EBAM process presents a challenge to the implementation of this technology. Ultrasound excitation applied during the EBAM process could improve the metal structure of the builds, thus making the components intrinsically better. The goal of this research is to determine if coupling an ultrasound source to the component during EBAM fabrication improves the subsequent metal structure. Successful outcome of this research could provide tangible improvements to this developing technology, by improving the resulting mechanical properties of the fabricated components. Many industries would benefit from the result. This project leverages existing technical competencies within Los Alamos and will ensure that the Laboratory remains a leader in the field of EBAM technology.

Technical Outcomes

An analytical method/instrumentation that improves mechanical properties of large 3-dimensional (3D) printed metal parts using Electron Beam Advance Manufacturing (EBAM). This is achieved through in-situ targeted acoustical excitation of the 3D printed part. The acoustics excitation is done at very specific frequencies, corresponding to natural resonances of the build, during the printing process (as the part is built).

Study for Alternative Cavity Wall and Inductive Insert Material

Charles Taylor
20210531MFR

Project Description

This research will seek to go beyond the limitations of longitudinal beam instability to the delivery of intense short-pulse beam to the Lujan center requested by both weapon stewardship neutron cross-section scientists and academic particle and nuclear physics researchers. The findings of this study – improving beam stability through alternative magnetic materials – would increase the amount of beam current that could be accumulated within the ring, thus permitting higher timing resolution studies. We expect the findings will offer insight into new possibilities for cavity designs and beamline construction, informing accelerator facility design and next-generation accelerators around the world.

Technical Outcomes

This study reviewed the key features of beam stability and has found solutions that will allow for finer beam time structure and increase beam currents to the experimental areas. We are currently working on publishing our results and we will continue to collaborate with other facilities struggling with similar issues. The team will design a new inductor for the Los Alamos Proton Storage Ring (PSR). Additionally, we are certain that other future Los Alamos Neutron Science Center (LANSCE) upgrades will profit from our findings.

Publications

Posters

Taylor, C. E. Study of Alternative Cavity Wall and Inductive Insert Material. Presented at *APS April Meeting 2021*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23352)

A Novel Heater Wire to Improve H- Ion Source Filament Lifetime

Prabir Roy
20210532MFR

Project Description

The Los Alamos Neutron Science Center (LANSCE) accelerator provides negative hydrogen ion (H-) beams to user facilities such as Proton Radiography (pRad), Ultra cold neutron source facility (UCN), Lujan Center (1L target), and Weapon Neutron Research (WNR). All of the user facilities receive H- beam pulses. A long-lasting heater filament is essential to provide beams. We intended to develop a filament that will last longer and produce electrons useful for interaction with Hydrogen plasma to make H-. Success will help bring new research & development on source-related material science to Los Alamos National Laboratory (LANL) and provide direct and immediate benefits to the current user programs at LANSCE by reducing accelerator down time. There is also international interest in an enhanced lifetime of such filaments. Thus, the results will also bolster the reputation of the Laboratory in the international accelerator physics community and may attract Department of Energy (DOE) Office of Science funding for ion source development.

Technical Outcomes

A morphology of tungsten (W) wire and wire of 3% Rhenium (Rh) mixed Tungsten (W) that is coated with Tantalum (Ta) for higher emission was conducted. It was observed that nominal tungsten wire grain size is elongated than the W-Rh wire, which may cause hotspot buildup. Therefore, it is expected that Rhenium mixed Tungsten wire may be helpful to increase wire elasticity, decrease hot spots, and increase filament's long lifetime.

Publications

Reports

Roy, P. K. A Novel Heater Wire to Improve H- Ion Source Filament Lifetime. Unpublished report. (LA-UR-21-27259)

Design for Manufacture Pit Feasibility Study (U)

Christina Scovel
20200665DI

Project Description

This project will produce one or more prototype pits that demonstrate Design for Manufacture (DfM) improvements, as well as develop an integrated certification and qualification plan for the example DfM pit. The DfM approach could result in substantial savings of money, time, and waste in future pit production processes. If this project is a success it will impact the design of the new plutonium facility and the national strategy for pit development.

Publications

Presentation Slides

Gubernatis, D. C. Design for Manufacturing (DfM) Engineers Week Presentation. Presented at *LANL Engineers Week 2021*, Los Alamos, New Mexico, United States, 2021-02-23 - 2021-02-25. (LA-UR-21-21564)

Mier, R. M. Rapid Prototyping of Forming Tools Through Additive Manufacturing. Presented at *DisrupTECH*, Los Alamos, New Mexico, United States, 2022-02-23 - 2022-02-23. (LA-UR-22-21011)

Casting: Design Responsiveness and Rapid Qualification

Kara Luitjohan
20210692DI

Project Description

The use of a cast part over a wrought (processed) part results in large savings in both time and money, therefore it is imperative to pursue approaches to control and optimize microstructural development during casting. This is critical for an agile, 21st century weapons complex. This project, by strengthening the processing-structure-property link in the area of solidification for uranium alloys, will allow new designs to be more responsive to mission needs. Furthermore, this will provide a significant step forward in being capable of designing for final properties while feeding back information on how to design components for ease of manufacturing. The broader mission of providing high quality uranium components for various research applications will also benefit from well-defined process-structure-property links.

Welding: Design Responsiveness and Rapid Qualification

Lindsay O'Brien
20210698DI

Project Description

The original welding and brazing methods and procedures used for pit production are being replaced rapidly due to new technology, aging of the materials used for decades, and more complete welding and joining science. New scientific approaches need to be developed in order to keep up with the programmatic demands for appropriately radiused test objects, future pit designs, and modifications to current designs. These same approaches are necessary in order to enhance legacy welds using new welding techniques and materials while still producing high quality, useful components. By utilizing the knowledge from past developments, including those from stockpile components, and combining it with modern techniques, such as blue light laser coordinate scanning, 3-Dimensional modeling, and finite element analysis, a method for accounting for weld distortion and its effect on overall component dimensions will be developed. A model for the deflection seen during welding will allow for more straightforward use of welding for test objects and more straightforward design changes in the future.

Powder Materials: Design Responsiveness and Rapid Qualification (U)

Kendall Hollis
20210699DI

Project Description

This research advances the agile design, testing and manufacturing of Department of Energy (DOE) relevant materials and applications. Three-dimensional (3D) printing is used to bring modern advances to the production of powder processed materials. This will apply to all materials and parts produced by cold isostatic pressing.

The Effect of Defects on the Plutonium Gallium (PuGa) Phase Boundaries (U)

Donald Brown
20210791DI

Project Description

As Plutonium Gallium (PuGa) components age in our enduring stockpile, spontaneous fission (alpha decay) events deposit defects in the microstructure. As in all metal alloys, these defects control the strength properties of PuGa and also effect the kinetics of phase transformations, potentially creating uncertainty in performance. This experimental work will collect data aimed at better understanding the effect of the defects on the phase transformations for the purpose of validating the development of microstructure aware models to be used in future performance calculations. Specifically, the delta-alpha transformation temperature will be determined with and without defects and the initiation sites for transformation will be directly observed. Also valuable equation of state data, i.e., the crystallographic thermal expansion, which is known to be hysteretic (depending on defects) will be determined over the measurement range.

New Technique for Uranium Hydride Analysis using Ultracold Neutrons

Zhaowen Tang
20210797DI

Project Description

Hydride formation in metals can lead to embrittlement of the material causing reduced ductility, decreased toughness, and fracture. Hydride formation in uranium (U) metal is particularly undesirable because it causes a 70% volume expansion of the metal lattice and the hydride corrosion product uranium hydride (UH_3) is a friable, pyrophoric powder. We propose to use Ultracold Neutrons (UCNs) to probe surface hydrogen (H) distribution and accumulation, helping us to discern whether UH_3 preferentially forms at the oxide/metal interface or in U metal, away from the interface. If these experiments are successful, the apparatus will also provide an important tool to study the effect of manufacturing process (e.g. various solidification technologies vs. wrought processing) on hydride corrosion susceptibility. A successful demonstration of this technique will be of interest to the National Nuclear Security Administration. The technique can also be expanded to other Uranium-based molecules, which will provide valuable data on surface hydride formation for nuclear fuel materials.

Publications

Presentation Slides

Ito, T. UCN Future at LANSCE. Presented at *LANSCE Future Spring Workshop*, Los Alamos, New Mexico, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-24476)

An Investigation of Variables Affecting Plutonium Hydriding (U)

Troy Holland
20210946DI

Project Description

Our nuclear materials models are critical to enable efficient design decisions that maintain the safety, security, and reliability of the stockpile. Lack of adequate models moves some stockpile stewardship activities to the realm of impossible or prohibitively difficult/expensive. Conversely, adequate computational models make necessary stockpile stewardship goals both possible and cost effective, while simultaneously keeping the nation's scientific capabilities as a whole at the global forefront.

Publications

Reports

Elliott, S. M. and T. M. Holland. Mechanisms and Isotope Effects in the Reverse Water Gas Shift. Unpublished report. (LA-UR-21-28598)

Novel in situ Probes of Mesoscale Materials Dynamics

Dmitry Yarotski
20190643DI

Project Description

Understanding materials behavior at the mesoscale is central to designing and realizing new material functionality. Recent advances in X-ray light sources are enabling significant increases in photon flux and coherency that are poised to provide novel insights into the microscopic origins of materials behavior with unprecedented temporal and spatial resolution, high element specificity and sensitivity to buried interfaces. The overarching goal of this project is to apply novel time-resolved in-situ X-Ray techniques to track materials properties under extreme environments of pressure, temperature and magnetic field. Our research efforts are organized in four crosscutting thrusts aimed at: (i) understanding and manipulating ultrafast magnetic dynamics induced by coherent infrared pulses; (ii) ultra-high-speed monitoring of microstructure and property evolution during additive manufacturing process; (iii) probing materials transformations at high pressures, temperatures and strain rates enabled by unique design of pressure cells; and (iv) developing automated real-time data analysis tools for steering the experiments at novel high-repetition rates light sources. We strongly believe that by pursuing these thrusts simultaneously, we will address the most compelling questions in current materials science using the most advanced techniques available to research community, and provide the Laboratory with a vital capability for probing broad range of mission-relevant materials.

Technical Outcomes

The team applied novel in-situ time- and space-resolved X-Ray techniques to enable significant advances in understanding of mesoscale phenomena underpinning magnetic, electronic, structural and micro-mechanical materials responses to extreme environments. Simultaneous pursuit of entangled research thrusts enabled us to jump start Los Alamos' efforts at novel coherent light sources and foster broad collaborations and synergies, both internal to the Laboratory and externally, that will lay the foundation for further activities in mesoscale materials science.

Publications

Journal Articles

Biwer, C. M., A. Quan, L. Q. Huston, B. Sturtevant and C. M. Sweeney. Real-time Tools for Analysis of Dynamic Diamond Anvil Cell Experiment Data. Submitted to *Review of Scientific Instruments*. (LA-UR-20-27493)

Biwer, C. M., D. R. Finstad, S. C. Vogel, J. Zhang, M. McKerns, N. S. Johnson and J. P. Ahrens. Spotlight: Automation of Rietveld Analyses Using an Ensemble of Local Optimizations on Distributed-Computing Networks. Submitted to *Journal of Applied Crystallography*. (LA-UR-20-27665)

Carr, A. V., J. M. Bowlan, C. Mazzoli, A. Barbour, W. Hu, S. Wilkins, C. Walker, X. Ding, N. Lee, J. H. Kim, Y. J. Choi, S. Lin, R. L. Sandberg and V. Zapf. Evidence for the Alternating Next-Nearest Neighbor model in the dynamic behavior of a frustrated antiferromagnet. Submitted to *Physical Review Letters*. (LA-UR-20-24289)

*Enriquez, E., G. Wang, Y. Sharma, I. Sarpkaya, Q. Wang, D. Chen, N. Winner, X. Guo, J. Dunwoody, J. White, A. Nelson, H. Xu, P. Dowden, E. Batista, H. Htoon, P. Yang, Q. Jia and A. Chen. Structural and Optical Properties of Phase-Pure UO , $\xce\xb1-U O$, and $\xce\xb1-UO$ Epitaxial Thin Films Grown by Pulsed Laser Deposition. 2020. *ACS Applied Materials & Interfaces*. **12** (31): 35232-35241. (LA-UR-20-24149 DOI: 10.1021/acsami.0c08635)

*Farmer, T. O., E. Guo, R. D. Desautels, L. DeBeer-Schmitt, A. Chen, Z. Wang, Q. Jia, J. A. Borchers, D. A. Gilbert, B. Holladay, S. K. Sinha and M. R. Fitzsimmons. Nanoscale magnetization inhomogeneity within single phase nanopillars. 2019. *Physical Review Materials*. **3** (8): 081401. (LA-UR-19-29646 DOI: 10.1103/PhysRevMaterials.3.081401)

Huston, L. Q., N. Velisavljevic, J. S. Smith, G. T. I. Gray and B. T. Sturtevant. Multi-phase equation of state of ultrapure hafnium to 120 GPa. 2022. *Journal of Physics: Condensed Matter*. **34** (5): 055401. (LA-UR-21-24396 DOI: 10.1088/1361-648X/ac33dd)

*Li, P., S. Maddali, A. Pateras, I. Calvo-Almazan, S. O. Hruszkewycz, W. Cha, V. Chamard and M. Allain. General approaches for shear-correcting coordinate transformations in Bragg coherent diffraction imaging. Part II. 2020. *Journal of Applied Crystallography*. **53** (2): 404-418. (LA-UR-20-21519 DOI: 10.1107/S1600576720001375)

Li, W., B. Zhu, Q. He, A. Y. Borisevich, C. Yun, R. Wu, P. Lu, Z. Qi, Q. Wang, A. Chen, h. wang, S. A. Cavill, K. H. Zhang and J. MacManus-Driscoll. Interface Engineered Room-Temperature Ferromagnetic Insulating State in Ultrathin Manganite Films. Submitted to *Advanced Sciences*. (LA-UR-20-24152)

*Li, W., B. Zhu, R. Zhu, Q. Wang, P. Lu, Y. Sun, C. Cafolla, Z. Qi, A. Chen, P. Gao, H. Wang, Q. He, K. Zhang and J. L. MacManus-Driscoll. Atomic-Scale Control of Electronic Structure and Ferromagnetic Insulating State in Perovskite Oxide Superlattices by Long-Range Tuning of BO Octahedra. 2020. *Advanced Functional Materials*. **30** (40): 2001984. (LA-UR-20-28256 DOI: 10.1002/adfm.202001984)

Pateras, A., R. Harder, W. Cha, J. G. Gigax, J. K. S. Baldwin, J. Tischler, R. Xu, W. Liu, M. Erdmann, R. Kalt, R. Sandberg, S. J. Fensin and R. Pokharel. Combining Laue diffraction with Bragg coherent diffraction imaging at 34-ID-C. Submitted to *Journal of Synchrotron Radiation*. (LA-UR-20-21980)

Pateras, A., R. Harder, W. Cha, J. G. Gigax, J. K. S. Baldwin, J. Tischler, R. Xu, W. Liu, M. Erdmannn, R. Kalt, R. L. Sandberg, S. J. Fensin and R. Pokharel. Combining Laue diffraction with Bragg coherent diffraction imaging at 34-ID-C. Submitted to *Journal of Synchrotron Radiation*. (LA-UR-20-25553)

*K. K. T. *. S. Y. *. N. H. *. Y. D. *. C. A. Paudel, B. *., B. Paudel, K. T. Kang, Y. Sharma, A. Chen and D. Yarotski. Symmetry mismatch controlled ferroelastic domain ordering and the functional properties of manganite films on cubic miscut substrates. 2021. *Physical Chemistry Chemical Physics*. **23** (31): 16623-16628. (LA-UR-21-29518 DOI: 10.1039/D1CP01957K)

*Paudel, B., I. Vasiliev, M. Hammouri, D. Karpov, A. Chen, V. Lauter and E. Fohtung. Strain charge mediated magnetoelectric coupling across the magnetic oxide/ferroelectric interfaces. 2019. *RSC Advances*. **9** (23): 13033-13041. (LA-UR-19-29648 DOI: 10.1039/C9RA01503E)

Paudel, B., K. T. Kang, Y. Sharma, H. Nakotte, D. A. Yarotski and A. Chen. Symmetry mismatch controlled ferroelastic domains ordering and functional properties of manganite films on cubic miscut substrates. Submitted to *Nanoscale*. (LA-UR-21-22621)

Sharma, Y., A. R. Mazza, B. L. Musico, E. Skoropata, R. Nepal, R. Jin, A. V. Ievlev, L. Collins, Z. Gai, A. Chen, M. Brahlek, V. Keppens and T. Z. Ward. Magnetic Texture in Insulating Single Crystal High Entropy Oxide Spinel Films. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-21-30189)

*Z. S. *. M. M. *. O. L. A. *. P. B. *. Y. D. *. H. J. *. C. A. *. H. B. D. Song, J. *., B. Paudel, A. Chen and D. Yarotski. Interfacial-Strain-Controlled Ferroelectricity in Self-Assembled BiFeO Nanostructures. 2021. *Advanced Functional Materials*. **31** (34): 2102311. (LA-UR-21-22846 DOI: 10.1002/adfm.202102311)

Reports

Sweeney, C. M., B. Sturtevant, C. M. Biwer, C. A. Bolme, R. C. Huber, L. Q. Huston, E. McBride, L. Miyagi, C. Prescher, K. J. Ramos, J. Smith and T. Turton. Data Science and Computation for Rapid and Dynamic Compression Experiment Workflows at Experimental Facilities Workshop Report. Unpublished report. (LA-UR-20-27469)

Presentation Slides

Carr, A. V., J. M. Bowlan, S. Lin, C. Mazzoli, A. Barbour, W. Hu, S. Wilkens, X. Ding, N. Lee, J. H. Kim, Y. J. Choi, R. L. Sandberg and V. Zapf. Traversing the "Devil's Staircase": Dynamic behavior of a frustrated antiferromagnet. Presented at *NSLS-II Friday Virtual Lunchtime Seminar Series (Webinar)*, Upton, New York, United States, 2020-12-04 - 2020-12-04. (LA-UR-20-29864)

Chen, A. Interplay of Strain, Defects and Interface on Functional Properties in Vertical Nanocomposites. Presented at *19th International Conference on Crystal Growth and Epitaxy (ICCGE-19)*, Keystone, Colorado, United States, 2019-07-28 - 2019-08-02. (LA-UR-19-27280)

Chen, A. Correlation among strain, defect, interface and functional properties in oxide nanocomposites. Presented at *CINT user meeting*, los alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27407)

Chen, J., N. E. Hahn and S. J. Fensin. Understanding the Role of Grain Boundary in Inducing Damage and Failure under Dynamic Loading in BCC Ta. Presented at *TMS 2020 Annual Meeting & Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21564)

Choi, Y. J. Applying Neural Networks to Experimental Diffraction Data. . (LA-UR-20-26201)

Huston, L. Q., E. K. Moss, J. S. Smith, R. Husband, Z. Jenei, H. P. Liermann, B. Sturtevant and E. F. O'bannon. Compression rate dependence of the α to ω phase transition in titanium. Presented at *ACA meeting 2020*, Virtual, New Mexico, United States, 2020-08-02 - 2020-08-02. (LA-UR-20-25893)

Huston, L. Q., E. K. Moss and B. Sturtevant. Dynamic Compression of Ti. . (LA-UR-20-23802)

Huston, L. Q., L. Miyagi, H. P. Liermann, R. Husband and B. Sturtevant. Radial diffraction in the dynamic DAC. Presented at *EuXFEL User Meeting*, Hamburg, Germany, 2020-01-29 - 2020-01-29. (LA-UR-20-20704)

Pandey, A. and R. Pokharel. Real-time analysis of diffraction data for enabling in-situ measurements. Presented at *TMS*

2020, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-22416)

Sturtevant, B. Proposal 2592: dDAC @ EuXFEL: "Ti Team" Kickoff Meeting. Presented at *Proposal 2592 Community Proposal Planning Meeting*, online, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20257)

Sturtevant, B., J. S. Pigott, L. Q. Huston, C. A. Bolme, D. M. Dattelbaum and H. Collaboration. Thermally-induced, quenchable bcc Zr using the European XFEL. Presented at *2020 European XFEL Users' Meeting*, Hamburg, Germany, 2020-01-27 - 2020-01-31. (LA-UR-20-20717)

Sweeney, C. M. Thrust IV: New Automated Real-Time Data Analysis and Data Management Tools. . (LA-UR-20-24282)

Sweeney, C. M. Data Science for Real-time Experimental Workflows at User Light Sources. . (LA-UR-21-24356)

Sweeney, C. M., A. Therrien and R. Coffee. Outbrief on LCLS Workshop on Automated Analysis and Control for X-ray Science. Presented at *High Power Laser Workshop*, Menlo Park, California, United States, 2019-09-26 - 2019-09-27. (LA-UR-19-30288)

Sweeney, C. M., C. M. Biwer and A. Quan. Tools and Workflow for Analysis of Dynamic Diamond Anvil Cell Experiment Data. Presented at *EuXFEL/DESY Users Meeting*, Hamburg, Germany, 2020-01-27 - 2020-01-31. (LA-UR-20-20709)

Posters

Huston, L. Q., L. Miyagi, H. P. Liermann, R. Husband and B. Sturtevant. Radial diffraction in the dynamic diamond anvil at ECB. Presented at *EuXFEL User Meeting*, Hamburg, Germany, 2020-01-29 - 2020-01-29. (LA-UR-20-20614)

Pateras, A., R. Harder, W. Cha, J. G. Gigax, J. K. S. Baldwin, J. Tischler, R. Xu, W. Liu, M. Erdmann, R. Kalt, R. L. Sandberg, S. J. Fensin and R. Pokharel. Novel X-ray Tools to Study Size Effects on Nanocrystalline Materials. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21520)

Other

Sturtevant, B., L. Q. Huston, A. Quan, C. M. Biwer and C. M. Sweeney. Data from Dynamic Diamond Anvil Cell Experiment October 2019. Dataset. (LA-UR-20-24551)

Expedited High Explosive Formulation Through Processing-structure-property-performance Relationships

Kyle Ramos
20200667DI

Project Description

After years of stockpile stewardship, we are in a period of "rapidly changing geopolitics wherein inter-state competition, not terrorism, is now the primary concern in United States national security [excerpt from Summary of the 2018 National Defense Strategy of the United States of America, Sharpening the American Military's Competitive Edge]." Laboratory scientists are being called upon to increase stockpile responsiveness. Our recent achievements in novel processing and pressing methods, using in situ diagnostics and sensors, and direct numerical simulation of plastic bonded explosives (PBXs) at the mesoscale, are reaching a state of maturity sufficient to greatly expedite formulation of high performance, reduced sensitivity PBX, with grain structures optimized for improving safety, mechanical properties, and manufacturability. With this materials science and engineering approach, the United States Nuclear Weapons complex can retain the performance and test history of high melting explosive (HMX)-based formulations such as PBX 9501 while still greatly improving them for use in the current and future stockpile.

Technical Outcomes

This project developed capabilities and processing-structure-property-performance relationships for expediting High Explosive formulation via modern manufacturing methods.

Publications

Journal Articles

Cawkwell, M. J., M. Zecevic, D. J. Luscher and K. J. Ramos. Dependence of the single crystal elastic constants of epsilon-CL-20, DAAF, FOX-7, beta-HMX, alpha-RDX, gamma-RDX, epsilon-RDX, and PETN on hydrostatic compression from dispersion-corrected density functional theory calculations. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-21-28923)

Cawkwell, M. J., M. Zecevic, D. J. Luscher and K. J. Ramos. Dependence of the elastic stiffness tensors of PETN, alpha-RDX, gamma-RDX, epsilon-RDX, epsilon-CL-20, DAAF, FOX-7, and beta-HMX on hydrostatic compression from dispersion-corrected density functional theory calculations.. Submitted to *Propellants, Explosives, Pyrotechnics*. (LA-UR-21-32458)

Cawkwell, M. J., N. Mohan, M. Zecevic, D. J. Luscher and K. J. Ramos. Structure and properties of dislocations and the twin boundary on (101) in beta-cyclotetramethylene tetranitramine. Submitted to *Philosophical Magazine*. (LA-UR-21-28916)

*Powell, M. S., D. S. Moore and S. D. McGrane. Insight into the chemistry of TNT during shock compression through ultrafast absorption spectroscopies. 2021. *The Journal of Chemical Physics*. **154** (5): 054201. (LA-UR-20-29986 DOI: 10.1063/5.0032018)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Simulating Knoop hardness anisotropy of Al and \xce \xb2-HMX with a crystal plasticity finite element model. Submitted to *International Journal of Plasticity*. (LA-UR-20-28670)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Crystal plasticity including a phase-field deformation twinning model for the high-rate deformation of cyclotetramethylene tetranitramine. Submitted to *Journal of the Mechanics and Physics of Solids*. (LA-UR-21-26956)

Reports

Powell, M. S., D. S. Moore and S. D. Mcgrane. Response to reviewers- Insight into The Chemistry of TNT During Shock Compression Through Ultrafast Absorption Spectroscopies. Unpublished report. (LA-UR-20-29987)

Saavedra, R. A., J. A. Matteson, K. A. Berchtold and K. J. Ramos. Design of a Slit Rheometer for Characterization of Explosive Formulations. Unpublished report. (LA-CP-20-20665)

Presentation Slides

Bolme, C. A., K. J. Ramos, M. J. Cawkwell, J. D. Lazarz, C. Liu, D. J. Luscher, S. D. Mcgrane, D. S. Moore, R. T. Perriot, M. S.

Powell, M. Zecevic and B. Zuanetti. HE Thermomechanics and High Strain Rate Loading. Presented at *PBX 9501 Conventional High Explosives Grand Challenge Symposium*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-10. (LA-UR-21-31863)

Cawkwell, M. J. Institutional Computing Report: Fast Quantum Molecular Dynamics with LATTE (w19_latteqmd). . (LA-UR-21-24031)

Powell, M. S. Insight into the chemistry of PETN and TNT during shock compression through ultrafast absorption spectroscopies. . (LA-UR-21-25141)

Powell, M. S., S. D. Mcgrane, R. T. Perriot, C. A. Bolme, D. S. Moore, J. D. Lazarz, M. J. Cawkwell and K. J. Ramos. Savannah River Seminar: Experimentally solving the heat equation. . (LA-UR-21-24515)

Powell, M. S., S. D. Mcgrane, R. T. Perriot, C. A. Bolme, D. S. Moore, M. J. Cawkwell and K. J. Ramos. Validating Thermomechanical Models with Stokes, anti-Stokes, Raman Thermometry and Impulsively Stimulated Light Scattering: Experimentally solving the heat equation. . (LA-UR-21-20024)

Powell, M. S., S. D. Mcgrane, R. T. Perriot, C. A. Bolme, D. S. Moore, M. J. Cawkwell and K. J. Ramos. Validating thermomechanical models of cyclotetramethylene tetranitramine (HMX) through impulsively stimulated thermal scattering. Presented at *March APS Meeting -- Virtual*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22177)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Single crystal model for high rate deformation of \xc3\x9f-HMX. Presented at *APS March Meeting 2021*, College Park, Maryland, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22333)

Zecevic, M., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Calibration of Dislocation Slip and Deformation Twinning Material Parameters for HMX. Presented at *USNCCM16 (16th U.S. National Congress on Computational Mechanics)*, Chicago, Illinois, United States, 2021-07-25 - 2021-07-29. (LA-UR-21-27313)

Posters

Liu, C., C. M. Cady and K. J. Ramos. Damage & Fracture of HE as a Function of Strain-Rate and Length-Scale. Presented at *2021 Conventional High Explosives Grand Challenge Technical Symposium - Mesoscale Physics Focus Session*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-10. (LA-UR-21-31735)

Morrow, B. M., C. E. Armenta and K. J. Ramos. Microstructural Characterization of HE and Mock Materials via Electron Microscopy Techniques. Presented at *2021 Conventional High Explosives Grand Challenge Technical Symposium*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-06. (LA-UR-21-31776)

Ramos, K. J., M. J. Cawkwell, D. J. Luscher, C. A. Bolme, C. E. Armenta, J. L. Barber, L. Dresselhaus-Marai, A. E. Gleason Holbrook, B. J. Jensen, H. J. Lee, I. Nam, P. A. Rigg, R. L. Sandberg, M. Seaberg and N. Sinclair. Developing and Validating Thermomechanics Models for Explosives with Experiments on Commensurate Scales. Presented at *PBX 9501 Conventional High Explosives Grand Challenge Symposium*, Los Alamos, New Mexico, United States, 2021-12-08 - 2021-12-08. (LA-UR-21-31821)

Investigation of the Role of Actinides on the Local Structure of Molten Salts Using Neutron Pair-distribution Function Analysis

Sven Vogel
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Project Description

Molten salts play important roles in nuclear processes from actinides processing (including spent fuel processing) to cooling or fuel media for novel reactor concepts (including small modular reactors). Properties of the melts are of paramount importance to understand, control, and optimize these processes and design for these applications. Due to the temperatures involved as well as chemical and radiological hazards involved, typical characterization techniques often cannot be applied. A information gap therefore exists to characterize these materials and in particular the influence of adding actinides, such as uranium (U) and plutonium (Pu), on the properties of the melts. While modeling can close some of these gaps, experimental data to benchmark these models is scarce. This proposal closes this gap by providing data on the pair-distribution function of the melts as a function of temperature and composition, including U and Pu. Assembling a team of experts in neutron characterization and molten salts and building on Los Alamos's unique capability to handle actinide-bearing samples, not available at other user facilities, we propose to use neutron pair-distribution function (PDF) analysis to characterize the local structure of molten salts in situ.

Technical Outcomes

The ability to safely collect data for neutron pair-distribution function (PDF) analysis of actinide-bearing molten salts was established and demonstrated by collection data for UCl3 in the molten state. In collaboration with external collaborators from Massachusetts Institute of Technology (MIT), data processing of the neutron scattering data to obtain the PDF from the collected data was established. The collaboration will continue, providing access for Los Alamos' to MIT's talent.

Publications

Journal Articles

Vogel, S. C., A. D. R. Andersson, M. J. Monreal, J. M. Jackson, S. S. Parker, G. Wang, P. Yang and J. Zhang. Crystal Structure Evolution of UCl3 from Room Temperature to Melting. Submitted to *JOM*. (LA-UR-21-24639)

Vogel, S. C., M. J. Monreal and A. P. Shivprasad. Materials for Small Nuclear Reactors and Micro Reactors, including Space Reactors. Submitted to *JOM*. (LA-UR-21-28723)

Presentation Slides

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

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

Accelerated Development of Additively Manufactured Uranium Oxide (UO2) Fuels for Geometries Avoiding Fuel Lifetime-limiting Irradiation Swelling Using Bulk Neutron Characterization

Bjorn Clausen
20200749DI

Project Description

In nuclear reactor environments, increasing burnup results in swelling of nuclear fuels due to the formation of fission gas bubbles and accumulation of solid fission products, limiting the achievable burnup and therefore the fuel economy. The use of fuel geometries other than sheets or cylinders can enhance geometrical stability at lower overall densities, which can mitigate the swelling, especially at ultra-high burnups. However, conventional fabrication techniques, especially for ceramic uranium dioxide (UO2) fuels, precluded development of such fuel forms. In recent years, significant development of advanced manufacturing technologies allows novel designs to overcome these limitations and fabricate fuel geometries that accommodate swelling much better, hence enabling higher burnup and therefore improve the economy of nuclear power generation. This project will leverage Los Alamos' unique characterization capabilities to advance this development, enabled by the pulsed neutron source at the Los Alamos Neutron Science Center, the high-energy X-ray computer tomography within the Non-Destructive Testing and Evaluation group, as well as existing Los Alamos infrastructure to handle nuclear materials. The non-destructive advanced characterization tools employed will for the first time give a complete picture of density and microstructure variations at the component length scale that can be used to optimize the manufacturing process.

Technical Outcomes

The project utilized unique Los Alamos' non-destructive neutron and X-ray techniques to characterization uranium dioxide (UO2) fuel pellets. The characterization is the presence of ~13 wt.% uranium carbon (UC) in the UO2 fuel, most likely from the sintering process, and the presence of local regions of higher attenuation in both samples observed with both X-rays and neutrons. These findings will aide Idaho National Laboratory in performing destructive testing in the regions identified as abnormal with our non-destructive characterization techniques.

Molecular Framework Architectures for Quantum Information

Jennifer Hollingsworth
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Project Description

Spins in molecules are a leading contender in the race for the next-generation qubit for quantum computing and quantum sensing. Spins have long coherence (phase memory) times, which means the operational time of a qubit made from them is also long. Spins can form entangled states, which means they could be used to create complex interacting networks of qubits. Both characteristics are key for envisioned quantum-enabled technologies. The next critical stage in the development of molecular quantum materials is to establish control over the spatial organization of molecular qubits without damaging the long coherence times they have as discrete molecules, as well as to create networks with deterministic and switchable interactions between qubits. This project will develop novel chemical frameworks for organizing and interacting molecular qubits, as well as underpinning knowledge for the predictive design of optimal frameworks for maximizing coherence and introducing precise and switchable control of qubit-qubit coupling.

Technical Outcomes

Molecular qubits were synthesized and chemically modified to enable assembly as metal-organic frameworks, with 8 metal–organic frameworks, including 6 new frameworks successfully assembled (goal 1) and electron-paramagnetic-resonance (EPR) spectroscopy confirming magnetic and/or qubit properties, with ability to interact geometrically or metal-identity-distinct qubit pairs (goal 2). Limited access to time-resolved-EPR prompted unexpected accomplishment-- building of system at Los Alamos. Modeling tools were established and benchmarked against experiment toward optimization of framework chemistry in large-scale assemblies for coherence and entanglement.

Publications

Presentation Slides

Dolgopolova, E. and J. A. Hollingsworth. Plasmonic spinel oxide nanocrystals afford Purcell-enhanced emission in the infrared. Presented at *ACS Spring 2021*, Online, New Mexico, United States, 2021-04-04 - 2021-04-30. (LA-UR-21-23397)

Enhancing Resonant Ultrasound Spectroscopy (RUS) to Measure the Elastic Properties of Complex Multi-Material Actinide Systems for In-Situ Applications

Timothy Ulrich
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Project Description

Elastic properties of materials are critical to provide confidence in a material to perform as expected. Current methodologies can provide accurate and precise properties, however, have strong limitations on their applicability, especially when the materials may be difficult to handle or be embedded in a larger system. Advances in both measurement technologies and computational capabilities now allow for extending current techniques to reduce or remove the current limitations. This project will enhance a current method known as resonant ultrasound spectroscopy by utilizing newly available techniques and provide a demonstration applied to a relevant actinide surrogate composite. This capability will greatly enhance nondestructive evaluation, manufacturing inspection and materials science with the ability to obtain the elastic properties of systems and in conditions where it is not currently possible to do so.

Technical Outcomes

This project was successful in extending resonant ultrasound spectroscopy to multi-material property determinations. This was demonstrated both numerically and experimentally using a variety of materials. In addition to the material properties of the materials, it was also established that the elastic properties of the thin elastic layer(s) connecting the materials can be determined using a similar methodology. Developments of this work are planned to be applied to composite systems for the weapons survivability program.

Publications

Journal Articles

Geimer, P. R., T. J. I. Ulrich, L. B. Beardslee, M. L. Hayne, M. Remillieux, T. A. Saleh and F. J. Freibert. Enhanced resonant ultrasound spectroscopy for measurement of the elastic properties of multi-material systems. Submitted to *Journal of the Acoustical Society of America*. (LA-UR-22-20167)

Presentation Slides

Geimer, P. R., T. J. I. Ulrich, M. Remillieux and L. B. Beardslee. Enhanced Resonant Ultrasound Spectroscopy for Multi-Material Characterization. Presented at *LANL Virtual Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27273)

I. Ulrich, T. J., M. Remillieux, L. B. Beardslee and P. Le Bas. Physical Acoustics Characterization For Inspection and Evaluation. . (LA-UR-21-24510)

Method for Extending the Plutonium-238 Supply

Kirk Weisbrod
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Project Description

The US requires plutonium-238 for nuclear stockpile program requirements and for powering NASA deep space and planetary missions. Currently the supply of suitable material is limited. If successful, this project will lead to development of a method that increases the availability of plutonium-238 for these missions. A limited scientific and engineering study will be performed to evaluate feasibility of a novel method, using materials and components that are already familiar to Plutonium Facility operators. Key modeling and experimentation will be completed to address the highest-risk aspects of the concept and provide estimates on productivity of a glovebox-scale system. Design for maintainability and impacts of radiolysis are explicit considerations.

Technical Outcomes

Initial operating parameters were developed for a system to increase the availability of plutonium-238 for nuclear stockpile programs and NASA deep space and planetary missions. The technical report provides robust estimates of the time required to produce a batch of product, the physical scale of the engineered system, and key radiolytic effects that must be managed for safe operation. An experimental path forward to reduce modeling uncertainty and initiate detailed engineering design is offered.

Rapid Actinide Identification via Luminescence (RAIL) Sensor

John Ahern
20210794DI

Project Description

Characterization of the diverse process solutions at Los Almaos National Laboratory's (LANL's) Plutonium Facility (PF-4) is a required step in processing material and inventory tracking for LANL missions. Analyzing more samples faster and with lower limits of detection would allow for less down time waiting on measurements, therefore more batches of product per year, which is vital to LANL missions. The central goal and anticipated outcome is a novel sensor system capable of simultaneously identifying and quantifying trace (<0.01 gram/Liter) selected actinides in simulated processing streams. This technology has broad impacts at LANL and beyond. This technology will improve the Lab's competitive position in developing sensor materials for improved process control. This is important to the Material Recycle and Recovery (MR&R) and Plutonium sustainment programs. If we succeed with our LDRD investment, we will deliver a new option that can be deployed, post-project, in an industrial-scale plutonium processing facility. LANL's Plutonium Facility (PF-4) is the only such complex in the United States and is designated as the "Plutonium Center of Excellence" by the National Nuclear Security Administration (NNSA).

Technical Outcomes

This project was successful in achieving the goal of identifying trace Americium and Uranium in simulated processing streams. Uranium was detected in 0.5 moles (M) nitric acid at ~0.010 grams/Liter without any sensitizing ligand or surfactant. This limit of detection is lower than expected for uranium without any sensitizing ligand. This has applications beyond the original aqueous processing streams. This could be useful for screening electrolyte solution for trace uranium after electrodecontamination of uranium parts.

Publications

Posters

Ahern, J. C., L. E. Wolfsberg, G. S. Goff and F. J. Freibert. Rapid Actinide Identification via Luminescence (RAIL) Sensor. Presented at *Actinide Separations Conference*, Richland, Washington, United States, 2021-05-18 - 2021-05-20. (LA-UR-21-24579)

Influence of Defects on the alpha to beta Phase Transformation in Plutonium

Sarah Hernandez
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Project Description

We currently have limited knowledge of the understanding of phase transformations, thermodynamics, and phase stability of plutonium (Pu) and knowing this information will help address future challenges in Pit Manufacturing, and inform related questions to equation of state within many programs, such as the Advanced Simulation and Computing (ASC) Physics and Engineering Model (PEM) Program. Furthermore, this fundamental project aims to enhance our basic knowledge of Pu phase transformations, and the results will provide an underlying fundamental scientific basis to future mission challenges pertaining to stockpile stewardship. Expected outcomes of the project will be a first-principles perspective of the influence of defects on the evolution and energetics required to undergo a phase transformation in Pu, which could either hinder or accelerate a phase transformation.

Technical Outcomes

Plutonium has a complex phase diagram, where the low-temperature phases are low-symmetry monoclinic structures and the mechanism for the alpha-beta phase transformation is not fully known. By using first-principles modeling and hypothesizing the role of defects (interstitials and vacancies), this project determined the possible mechanism for the alpha-beta phase transformation. Plutonium interstitials in alpha induced beta-like distortions, and vacancies located at atomic site-5 in beta were energetically lower in comparison to the alpha and delta-phases.

Publications

Journal Articles

Saxena, A. B., M. Porta, T. Castan and A. Planes. Flexocaloric effect near a ferroelastic transition. Submitted to *Physical Review B*. (LA-UR-21-25130)

Presentation Slides

Hernandez, S. C. Understanding an Unconventional Element Known as Plutonium. . (LA-UR-21-26157)

Hernandez, S. C. First-Principles Insights on the Phase Transformations of Pu. . (LA-UR-21-29081)

Hernandez, S. C. First-Principles Insights on the \xce \xb4\xe2\x86\x92\xce\xb1\xd5\x9b Martensitic Phase Transformations of Pu. . (LA-UR-21-30095)

Hernandez, S. C., S. K. Barman and S. B. Boden. Exploring the Metastability of Ga-stabilized \xce\xb4-Pu. . (LA-UR-22-22430)

Posters

Hernandez, S. C., S. B. Boden and A. B. Saxena. First-Principles Insights on the Phase Transformations of Pu. Presented at *Weapons System Capability Review*, Los Alamos, New Mexico, United States, 2021-08-24 - 2021-08-24. (LA-UR-21-28298)

Corrosion Protection of Plutonium using Atomic Armor

Doinita Neiner
20210796DI

Project Description

This project is aimed at a new concept to address plutonium metal oxidation or corrosion, namely the use of Atomic Armor in the form of graphene or graphene oxide coatings. Plutonium metal is a highly reactive metal that rapidly oxidizes. Oxidation or corrosion can be extremely detrimental to a process flow stream and product output within a manufacturing environment, can significantly influence the requirements for handling and storage of plutonium materials, and can impact the use of plutonium materials in a variety applications or scientific studies. This project is a small-scale, cutting-edge, high-risk and high pay-off project, that if successful will have applications across several plutonium science and technology areas. This project aims to characterize the materials from the corrosion experiments and develop ways to place the graphene oxide (GO) onto the metal substrate. If found to be successful, graphene or GO coatings will provide an alternate method to protect plutonium against oxidation and corrosion. This would have direct ties to not only actinide science, research and technology but would show particular relevance to the plutonium manufacturing mission.

Technical Outcomes

The project had the goal of characterizing the samples resulted from previous corrosion experiments, and develop a method to putting the graphene oxide (GO) membrane on the Plutonium (Pu) surface. Characterization data shows Pu is covered with the GO before and after the corrosion experiment. The identified deposition method allowed the team to perform another corrosion experiment.

Seaborg Institute: Center for Advancing Actinide Science and Technology at Los Alamos National Laboratory

Franz Freibert
20210527CR-GST

Project Description

The Glenn T. Seaborg Institute project goal is intended to promote cutting edge ideas in actinide science, research and technology development with a focus on actinide competency and capability development with international collaboration relevant to all areas of Los Alamos National Laboratory (LANL) actinide mission space. This effort intersects with nuclear energy, nuclear weapons, and global security and will address the outstanding problems being identified and championed within the LANL Actinide Strategy Initiative via providing short-term seed money for postdocs, early career scientists and engineers to initiate research aimed at providing the competency and technical underpinnings necessary for multi-year projects; fostering sustained excellence and enhanced external visibility in relevant science; and establishing an intellectual community to facilitate the nucleation of ideas to solve timely and important relevant mission scientific and technological problems. Stakeholder federal agencies for Los Alamos actinide mission include Department of Energy (DOE)/National Nuclear Security Administration (NNSA)/Defense Programs, DOE/NNSA/Nuclear Nonproliferation, National Aeronautics and Space Administration (NASA), Department of Homeland Security (DHS)/Domestic Nuclear Detection Office (DNDO) and Department of Health and Human Services (DHHS). Mission Relevance includes Nuclear Security and National Defense, Energy Security, Environmental Management, and overall scientific discovery and innovation.

Publications

Journal Articles

Abdul-Jabbar, N. M., T. Ulrich and J. T. White. Examination of phase equilibria in the carbon-titanium-titanium system for ultra-high temperature nuclear fuels. Submitted to *JOM*. (LA-UR-21-24633)

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

Carpenter, S. H., N. J. Wolford, B. S. Billow, M. T. Janicke, M. L. Neidig and A. Tondreau. Isolation and characterization of homoleptic uranium-bis(acyl)phosphine complexes. Submitted to *Inorganic Chemistry*. (LA-UR-21-24868)

Huston, L. Q., N. Velisavljevic, J. S. Smith, G. T. I. Gray and B. T. Sturtevant. Multi-phase equation of state of ultrapure hafnium to 120 GPa. 2022. *Journal of Physics: Condensed Matter*. **34** (5): 055401. (LA-UR-21-24396 DOI: 10.1088/1361-648X/ac33dd)

Huston, L. Q., S. C. Couper, M. Jacobsen, E. K. Moss, L. Miyagi, J. S. Smith, N. Velisavljevic and B. Sturtevant. Yield strength of CeO2 measured from static compression in a radial diamond anvil cell. Submitted to *Physical Review Materials*. (LA-UR-22-22048)

Kasper, J. M., X. Li, S. A. Kozimor, E. R. Batista and P. Yang. On the Relativistic Effects in Modeling the Ligand K-edge XANES of Uranium Complexes. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-21-25945)

Klamm, B. E., K. Bhardwaj, S. M. Greer, H. D. Root, S. Sharma, C. J. Windorff, M. M. MacInnes, S. H. Carpenter, T. E. Albrecht-Schonzart, B. L. Scott, B. Stein, S. A. Kozimor and A. Tondreau. Caging Plutonium. Submitted to *Inorganic Chemistry*. (LA-UR-21-28031)

V. R. K. *. K. K. K. *. K. D. *. S. Y. *. A. M. *. K. S. V. *. Z. M. Liu, Y. *. and Y. Sharma. Decoding the shift-invariant data: applications for band-excitation scanning probe microscopy. 2021. *Machine Learning: Science and Technology*. **2** (4): 045028. (LA-UR-21-24955 DOI: 10.1088/2632-2153/ac28de)

MacInnes, M. M., Z. R. Jones, N. H. Anderson, C. Eiroa Lledo, M. Y. Livshits, S. A. Kozimor, V. Mocko, F. Rein Rocha, B. Stein, K. E. Knope and J. N. Wacker. Using Molten Salts to Probe Outer-Coordination Sphere Effects on Lanthanide(III/II) Electron-Transfer Reactions. Submitted to *Journal of the American Chemical Society*. (LA-UR-21-25246)

O'Brien, M. K. Mary O'Brien Women in Engineering Profile. Submitted to *Advanced Materials & Processes*. (LA-UR-22-22247)

Paudel, B., Y. Sharma, B. K. Derby, G. Pilania, M. M. Schneider, A. C. Jones, H. Nakotte, M. T. Pettes and A. Chen. Effect of Lattice Strain on Magnetism in Epitaxial YCrO3 Films. Submitted to *APL Materials*. (LA-UR-21-24953)

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

Schlimgen, A. W., P. Yang and E. R. Batista. Excited States, Ionization Energies, and Electron Correlation for PuO2 Using DMRG with Large Active Spaces. Submitted to *Journal of Chemical Physics*. (LA-UR-21-21239)

Sharma, Y., A. R. Mazza, B. L. Musico, E. Skoropata, R. Nepal, R. Jin, A. V. Ievlev, L. Collins, Z. Gai, A. Chen, M. Brahlek, V. Keppens and T. Z. Ward. Magnetic Texture in Insulating Configurationally-Complex Single Crystal Spinel Films. Submitted to *Advanced Functional Materials*. (LA-UR-21-24957)

Sharma, Y., B. Paudel, J. Lee, W. S. Choi, Z. Yang, H. Wang, Y. Du, K. T. Kang, G. Pilania and A. Chen. Tuning magnetic and optical properties through strain in epitaxial LaCrO3 thin films. Submitted to *Physical Review Materials*. (LA-UR-21-20416)

*Sharma, Y., E. Skoropata, B. Paudel, K. T. Kang, D. Yarotski, T. Z. Ward and A. Chen. Epitaxial Stabilization of Single-Crystal Multiferroic YCrO3 Thin Films. 2020. *Nanomaterials*. **10** (10): 2085. (LA-UR-20-29015 DOI: 10.3390/nano10102085)

Sharma, Y., M. C. Lee, K. Pitike, K. K. Mishra, Q. Zheng, X. Gao, B. L. Musicao, A. R. Mazza, R. S. Katiyar, V. Keppens, M. Brahlek, D. A. Yarotski, R. P. Prasankumar, A. Chen, V. R. Cooper and T. Z. Ward. High Entropy Oxide Relaxor Ferroelectrics. Submitted to *ACS-JACS*. (LA-UR-21-24954)

Presentation Slides

Carpenter, S. H. Structure, Reactivity, and Electronic Structure Studies of f-Block Elements with Phosphorus Containing Ligands. Presented at *Actinide Lecture Series*, Los Alamos, New Mexico, United States, 2021-03-18 - 2021-03-18. (LA-UR-21-22765)

Carpenter, S. H. Structure, Reactivity, and Electronic Structure Studies of f-Block Elements with Phosphorus Containing Ligands. Presented at *ACS Spring Meeting*, Los Alamos, New Mexico, United States, 2021-04-05 - 2021-04-30. (LA-UR-21-23284)

Freibert, F. J. Actinide ST&E Strategic Investments. Presented at *Weapons Systems Capability Review Actinide Science and Manufacturing*, Los Alamos, New Mexico, United States, 2021-08-23 - 2021-08-26. (LA-UR-21-28256)

Murillo, J. MS 0765 Plutonium amide molecular structure. . (LA-UR-21-29086)

Schlimgen, A. W., E. R. Batista and P. Yang. Correlated Electronic Structure of Molecular PuO20/+1/+2: Large Active-Space Calculations with DMRG and Entanglement Measures. . (LA-UR-20-29421)

Schoenemann, R. U. Magnetoelastic Standing Waves Induced in UO2 by Microsecond Magnetic Field Pulses. Presented at *Actinide Science Lecture*, Los Alamos, New Mexico, United States, 2020-10-29 - 2020-10-29. (LA-UR-20-28729)

Schoenemann, R. U. Thermal and magnetoelastic properties of \xce\xb1-RuCl3 in the field-induced low temperature states. Presented at *ARHMF 2020*, Tohoku, Japan, 2020-12-01 - 2020-12-03. (LA-UR-20-29865)

Schoenemann, R. U. FBG techniques at the MAGLAB. Presented at *FBG strain gauge meet up*, Tokyo, Japan, 2021-02-22 - 2021-02-22. (LA-UR-21-21662)

Schoenemann, R. U. Thermal and magnetoelastic properties of \xce\xb1-RuCL3 in the field induced low temperature states. Presented at *APS March Meeting 2021*, Nashville, Tennessee, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22599)

Stein, B. Excited State Properties of Lanthanide TTA Complexes. Presented at *BES HEC Contractor meeting (virtual)*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25235)

van Veelen, A., S. M. Hickam, A. L. Pugmire, J. R. Bargar, N. P. Edwards and S. M. Webb. X-ray molecular signatures of UO2 chemical processing for Nuclear Forensic Science. Presented at *ACS Fall Meeting*, Atlanta, Georgia, United States, 2021-08-22 - 2021-08-26. (LA-UR-21-28453)

Other

Freibert, F. J. Glenn T. Seaborg, the US DOE Complex Actinide Mission, and the Seaborg Institute Network. Audio/Visual. (LA-UR-21-25387)

Schlimgen, A. W. Dataset of ab initio calculations on lanthanide and actinide molecules. Dataset. (LA-UR-21-21925)

Theory and Computation on Quantum Systems

Angel Garcia
20190495CR-CNL

Project Description

This project addresses fundamentals of the electronic properties of materials, from actinides to photovoltaics, with emphasis on computational algorithms. We will apply concepts and algorithms of quantum computation to (1) understand the electronic structure of materials from complex correlated systems (2) explore novel functionality in topologically protected states, and (3) Explore new quantum computing algorithms to solve optimization problems in quantum computers and/or annealers. This work has relevance in developing new materials for energy applications, modeling and predicting properties of f-electron matter, including plutonium, for National Nuclear Security Administration mission objectives, and developing materials for quantum computing applications.

Technical Outcomes

This project focused on the development of theories, theoretical methods, and models that provide an accurate description of physical systems where the quantum effects have a dominating role in their behavior. The project supported postdoctoral fellows, students and visitors working in the area of theory and computation of quantum systems. The scientific performance in this project has been truly outstanding, with 141 published papers in three years.

Publications

Journal Articles

Arrasmith, A. T., Z. P. Holmes, M. V. S. Cerezo de la Roca and P. J. Coles. Equivalence of quantum barren plateaus to cost concentration and narrow gorges. Submitted to *Quantum Science and Technology (QST)*. (LA-UR-21-23454)

*Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihalak. Near-gathering of energy-constrained mobile agents. 2021. *Theoretical Computer Science*. **849**: 35-46. (LA-UR-19-23906 DOI: 10.1016/j.tcs.2020.10.008)

Beckey, J. L., N. Gigena, P. J. Coles and M. V. S. Cerezo de la Roca. A computable and operationally meaningful multipartite entanglement monotone. Submitted to *Physical Review Letters*. (LA-UR-21-23423)

Beckey, J., A. Sone, M. V. S. Cerezo de la Roca and P. J. Coles. Variational Quantum Fisher Information Estimation. Submitted to *Quantum*. (LA-UR-20-28328)

Bilkis, M., M. V. S. Cerezo de la Roca, G. Verdon, P. J. Coles and L. Cincio. A semi-agnostic ansatz with variable structure for quantum machine learning. Submitted to *Quantum*. (LA-UR-21-22040)

Bravo-Prieto, C., R. LaRose, M. V. S. Cerezo de la Roca, Y. Subasi, L. Cincio and P. J. Coles. Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems. Submitted to *arXiv*. (LA-UR-19-29101)

Caro, M., H. Huang, M. V. S. Cerezo de la Roca, K. Sharma, A. T. Sornborger, L. Cincio and P. J. Coles. Generalization in quantum machine learning from few training data. Submitted to *Nature Physics*. (LA-UR-21-31086)

Caro, M., L. Cincio, J. Gibbs, Z. P. Holmes, N. A. Ezzell, H. Huang, A. T. Sornborger and P. J. Coles. Dynamical simulation via quantum machine learning with provable generalization. Submitted to *PRL*. (LA-UR-22-20965)

Cerezo, M., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation. 2020. *Quantum*. **4**: 248. (LA-UR-19-25585 DOI: 10.22331/q-2020-03-26-248)

*Cerezo, M., A. Sone, T. Volkoff, L. Cincio and P. J. Coles. Cost function dependent barren plateaus in shallow parametrized quantum circuits. 2021. *Nature Communications*. **12** (1): 1791. (LA-UR-19-32681 DOI: 10.1038/s41467-021-21728-w)

Ezzell, N. A., Z. P. Holmes and P. J. Coles. Minimal distance of quantum states with a rank constraint. Submitted to *Quantum Journal*. (LA-UR-22-21834)

Fontana, E., M. V. S. Cerezo de la Roca, A. T. Arrasmith, I. Runnger and P. J. Coles. Optimizing parameterized quantum circuits via noise-induced breaking of symmetrie. Submitted to *Quantum*. (LA-UR-20-29359)

Gao, X., F. Ramezanghorbani, J. S. Smith and A. E. Roitberg. TorchANI: A Free and Open Source PyTorch Based Deep Learning Implementation of the ANI Neural Network Potentials. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22710)

Ghosh, D., A. J. Neukirch and S. Tretiak. Light Emission in 2D Bromide Perovskites : Spacer Cations Matter. Submitted to *Nano Letters*. (LA-UR-19-31189)

Ghosh, D., D. Acharya, L. Pedesseau, C. Katan, J. Even, S. Tretiak and A. J. Neukirch. Charge Carrier Dynamics in Two-Dimensional Lead Iodide Perovskites: Dion-Jacobson vs. Ruddlesden-Popper Phases. Submitted to *ACS Nano*. (LA-UR-20-25290)

*Ghosh, D., D. Acharya, L. Zhou, W. Nie, O. V. Prezhdo, S. Tretiak and A. J. Neukirch. Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. 2019. *The Journal of Physical Chemistry Letters*. **10** (17): 5000-5007. (LA-UR-19-26501 DOI: 10.1021/acs.jpclett.9b02020)

Ghosh, D., E. Welch, A. J. Neukirch, A. Zakhidov and S. Tretiak. Polarons in Halide Perovskites: A Perspective. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-31317)

Ghosh, D., M. Rahil, P. Rajput and S. Ahmad. Highly Tunable Single Phase Excitons in KI Doped Organo-Lead Bromide Layered Perovskites. Submitted to *Chemistry of Materials*. (LA-UR-20-23374)

Gifford, B. J., A. Saha, B. M. Weight, X. He, G. Ao, M. Zheng, H. Htoon, S. Kilina, S. K. Doorn and S. Tretiak. Mod(n-m,3) Dependence of Defect-State Emission Bands in Aryl Functionalized Carbon Nanotubes. Submitted to *Nature Communications*. (LA-UR-19-26231)

Gifford, B. J., S. Kilina, H. Htoon, S. K. Doorn and S. Tretiak. Controlling Defect-State Photophysics in Covalently Functionalized Single-Walled Carbon Nanotubes. Submitted to *Accounts of Chemical Research*. (LA-UR-20-28343)

*Gifford, B. J., X. He, M. Kim, H. Kwon, A. Saha, A. E. Sifain, Y. Wang, H. Htoon, S. Kilina, S. K. Doorn and S. Tretiak. Optical Effects of Divalent Functionalization of Carbon Nanotubes. 2019. *Chemistry of Materials*. **31** (17): 6950-6961. (LA-UR-18-31887 DOI: 10.1021/acs.chemmater.9b01438)

Gifford, B. J. and S. Kilina. Contribution of Alkyl Side Chains to Chirality Sensitive Interactions between Single Walled Carbon Nanotubes and Polyfluorenes. Submitted to *Carbon*. (LA-UR-19-23831)

Gonzalez, D. G., G. Wang, P. Yang and E. R. Batista. First-principle modeling of the conductivity at the SrTiO3/LaAlO3 heterointerface on the 001, 110 and 111 planes. Submitted to *Physical Review B*. (LA-UR-21-29074)

Holmes, Z. P., A. T. Arrasmith, B. Yan, P. J. Coles, A. Albrecht and A. T. Sornborger. Barren plateaus preclude learning scramblers. Submitted to *Physical Review Letters*. (LA-UR-20-27596)

Holmes, Z. P., K. Sharma, M. V. S. Cerezo de la Roca and P. J. Coles. Connecting ansatz expressibility to cost gradients and barren plateau. Submitted to *Quantum*. (LA-UR-21-20034)

Larocca, M., P. J. Czarnik, K. Sharma, G. Muraleedharan, P. J. Coles and M. V. S. Cerezo de la Roca. Diagnosing barren plateaus with tools from quantum optimal control. Submitted to *Physical Review X Quantum*. (LA-UR-21-24973)

*Li, S., Y. Su, Y. Ren and L. He. Valley Polarization and Inversion in Strained Graphene via Pseudo-Landau Levels, Valley Splitting of Real Landau Levels, and Confined States. 2020. *Science*. **124** (10): 106802. (LA-UR-19-21456 DOI: 10.1103/PhysRevLett.124.106802)

*Liu, Y., Y. Su, X. Zhou, L. Yin, C. Yan, S. Li, W. Yan, S. Han, Z. Fu, Y. Zhang, Q. Yang, Y. Ren and L. He. Tunable Lattice Reconstruction, Triangular Network of Chiral One-Dimensional States, and Bandwidth of Flat Bands in Magic Angle Twisted Bilayer Graphene. 2020. *Physical Review Letters*. **125** (23): 236102. (LA-UR-20-24943 DOI: 10.1103/PhysRevLett.125.236102)

*Lovell, A., A. Mohan, P. Talou and M. Chertkov. Constraining Fission Yields Using Machine Learning. *EPJ Web of Conferences*. **211**: 04006. (LA-UR-18-30827 DOI: 10.1051/epjconf/201921104006)

Malla, R. K., A. B. Saxena and W. J. de Melo Kort-Kamp. Emerging nonlinear Hall effect in Kane-Mele two-dimensional topological insulators. Submitted to *Physical Review B*. (LA-UR-21-28047)

Malla, R. K., V. Y. Chernyak and N. Sinitsyn. Nonadiabatic transitions in Landau-Zener grids: integrability and semiclassical theory. Submitted to *Physical Review B*. (LA-UR-21-20136)

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear photonics of topological Dirac fermions in spin-orbit coupled graphene family materials. Submitted to *Communications physics*. (LA-UR-20-30407)

Pesah, A., M. V. S. Cerezo de la Roca, S. Wang, T. J. Volkoff, A. T. Sornborger and P. J. Coles. Absence of Barren Plateaus in Quantum Convolutional Neural Network. Submitted to *Physical Review X*. (LA-UR-20-29031)

S. Cerezo de la Roca, M. V., A. Sone, J. Beckey and P. J. Coles. A Generalized Measure of Quantum Fisher Information. Submitted to *Physical Review A*. (LA-UR-20-27870)

S. Cerezo de la Roca, M. V., A. Sone, J. L. Beckey and P. J. Coles. Sub-Quantum Fisher Information. Submitted to *Physical Review Letters*. (LA-UR-21-20536)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, P. J. Czarnik, L. Cincio and P. J. Coles. Effect of barren plateaus on gradient-free optimization. Submitted to *Quantum*. (LA-UR-20-29699)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio and P. J. Coles. Variational Quantum Algorithms. Submitted to *Nature Reviews Physics*. (LA-UR-20-30142)

S. Cerezo de la Roca, M. V., K. Sharma, A. T. Arrasmith and P. J. Coles. Variational Quantum State Eigensolver. Submitted

to *Nature Partner Journal Quantum Information*. (LA-UR-20-22660)

S. Cerezo de la Roca, M. V. and P. J. Coles. Impact of Barren Plateaus on the Hessian and Higher Order Derivatives. Submitted to *Physical Review A*. (LA-UR-20-26309)

*Rybin, N., D. Ghosh, J. Tisdale, S. Shrestha, M. Yoho, V. Duc, J. Even, C. Katan, W. Nie, A. J. Neukirch and S. Tretiak. Effects of Chlorine Mixing on Optoelectronics, Ion Migration, and Gamma-Ray Detection in Bromide Perovskites. 2020. *Advanced Materials*. **32** (5): 1854-1863. (LA-UR-19-29200 DOI: 10.1021/acs.chemmater.9b04244)

Saxena, A. B. and J. Cen. Anti-PT-symmetric qubit: Decoherence and entanglement entropy. Submitted to *Physical Review A*. (LA-UR-20-26138)

Schatzki, L., M. V. S. Cerezo de la Roca, A. T. Arrasmith and P. J. Coles. Entangled Datasets for Quantum Machine Learning. Submitted to *Physical Review X Quantum*. (LA-UR-21-28803)

Sharma, K., M. V. S. Cerezo de la Roca, L. Cincio and P. J. Coles. Trainability of Dissipative Perceptron-Based Quantum Neural Networks. Submitted to *Physical Review Letters*. (LA-UR-20-23484)

Sharma, K., M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio, A. T. Sornborger and P. J. Coles. Reformulation of the No-Free-Lunch Theorem for Entangled Data Sets. Submitted to *Nature Physics*. (LA-UR-20-25010)

*Sharma, K., S. Khatri, M. Cerezo and P. J. Coles. Noise resilience of variational quantum compiling. 2020. *New Journal of Physics*. **22** (4): 043006. (LA-UR-19-28095 DOI: 10.1088/1367-2630/ab784c)

Sifain, A. E., L. A. Lystrom, R. A. Messerly, J. S. Smith, B. T. Nebgen, K. M. Barros, S. Tretiak, N. E. Lubbers and B. J. Gifford. Predicting Phosphorescence and Inferring Wavefunction Localization with Machine Learning. Submitted to *Chemical Science*. (LA-UR-21-21632)

*Smith, J. S., B. T. Nebgen, R. Zubatyuk, N. Lubbers, C. Devereux, K. Barros, S. Tretiak, O. Isayev and A. E. Roitberg. Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. 2019. *Nature Communications*. **10** (1): 2903. (LA-UR-18-25687 DOI: 10.1038/s41467-019-10827-4)

Smith, J. S., C. Devereux, K. K. Davis, R. Zubatyuk, K. M. Barros, O. Isayev and A. E. Roitberg. Extending the applicability of the ANI deep learning molecular potential to Sulfur and Halogens. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-20841)

Smith, J. S., N. E. Lubbers, A. P. Thompson and K. M. Barros. Simple and efficient algorithms for training machine learning potentials to force data. Submitted to *Journal of Chemical Physics*. (LA-UR-20-24120)

*Smith, J. S., R. Zubatyuk, B. Nebgen, N. Lubbers, K. Barros, A. E. Roitberg, O. Isayev and S. Tretiak. The ANI-1ccx and ANI-1x

data sets, coupled-cluster and density functional theory properties for molecules. 2020. *Scientific Data*. **7** (1): 134. (LA-UR-19-29769 DOI: 10.1038/s41597-020-0473-z)

Sone, A., Y. Liu and P. Cappellaro. Quantum Jarzynski equality of open quantum systems in one-time measurement scheme. Submitted to *Physical Review Letters*. (LA-UR-19-32640)

Sone, A. and S. Deffner. Jarzynski equality for conditional stochastic work. Submitted to *Journal of Statistical Physics*. (LA-UR-20-28110)

Sone, A. and S. Deffner. Quantum and classical ergotropy from relative entropies. Submitted to *Physical Review Letters*. (LA-UR-21-22722)

Sornborger, A. T., B. A. Commeau, M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio and P. J. Coles. \xef\xbb\xbfVariational Hamiltonian Diagonalization for Dynamical Quantum Simulation. Submitted to *Quantum*. (LA-UR-20-26827)

Su, Y., A. Masaki-Kato, W. Zhu, J. Zhu, Y. Kamiya and S. Lin. Stable Higgs mode in anisotropic quantum magnets. Submitted to *Physical Review X*. (LA-UR-20-24832)

*Su, Y. and S. Lin. Current-Induced Reversal of Anomalous Hall Conductance in Twisted Bilayer Graphene. 2020. *Physical Review Letters*. **125** (22): 226401. (LA-UR-20-21206 DOI: 10.1103/PhysRevLett.125.226401)

Su, Y. and S. Lin. Topological Sliding Moire \xcc\x81 Heterostructure. Submitted to *Physical Review Letters*. (LA-UR-19-30658)

Talapatra, A. A., D. Ghosh, B. P. Uberuaga and G. Pilania. Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. 2021. *Journal of Materials Science*. **56** (28): 15812-15823. (LA-UR-21-23719 DOI: 10.1007/s10853-021-06294-2)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. 2022. *Physical Review Letters*. **128** (1): 010401. (LA-UR-21-20437 DOI: 10.1103/PhysRevLett.128.010401)

Tretiak, S., H. N. Yuvero, A. Mukazhanova, S. Sharifzadeh, V. M. Freixas and S. Fernandez-Alberti. Vibronic photoexcited dynamics of perylene diimide: computational insights. Submitted to *Journal of Physical Chemistry C*. (LA-UR-21-29026)

Tretiak, S., J. F. Galindo, V. M. Freixas and S. Fernandez-Alberti. Back-and-forth energy transfer during electronic relaxation in a chlorin-perylene dyad. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-29025)

Tretiak, S., M. Bhati, S. A. Ivanov and D. Ghosh. Nature of Electronic Excitations in Non-stoichiometric Quantum Dots. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-27876)

*Di Tullio, M., R. Rossignoli, M. Cerezo and N. Gigena. Fermionic entanglement in the Lipkin model. 2019. *Physical Review*

A. **100** (6): 062104. (LA-UR-19-27998 DOI: 10.1103/ PhysRevA.100.062104)

Wang, S., E. Fontana, M. Cerezo, K. Sharma, A. Sone, L. Cincio and P. J. Coles. Noise-induced barren plateaus in variational quantum algorithms. 2021. *Nature Communications*. **12** (1): 6961. (LA-UR-20-25526 DOI: 10.1038/s41467-021-27045-6)

*Wang, Z., Y. Su, S. Lin and C. D. Batista. Skyrmion Crystal from RKKY Interaction Mediated by 2D Electron Gas. 2020. *Physical Review Letters*. **124** (20): 207201. (LA-UR-19-31876 DOI: 10.1103/PhysRevLett.124.207201)

Weight, B. M., A. E. Sifain, B. J. Gifford, D. S. Kilin, S. Kilina and S. Tretiak. Coupling between Emissive-Defects of Carbon Nanotubes: Modeling Insights. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-24965)

Weight, B. M., A. E. Sifain, B. J. Gifford, D. S. Kilin, S. Kilina and S. Tretiak. Coupling between Emissive-Defects of Carbon Nanotubes: Modeling Insights. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-21-24965)

Weight, B. M., B. J. Gifford, S. Tretiak and S. Kilina. Interplay between Electrostatic Properties of Molecular Adducts and Their Positions at Carbon Nanotubes. Submitted to *Journal of Physical Chemistry C*. (LA-UR-21-21212)

*Yan, B., V. Y. Chernyak, W. H. Zurek and N. A. Sinitsyn. Nonadiabatic Phase Transition with Broken Chiral Symmetry. 2021. *Physical Review Letters*. **126** (7): 070602. (LA-UR-20-26742 DOI: 10.1103/PhysRevLett.126.070602)

Yan, B. and N. Sinitsyn. Recovery of damaged information and the out-of-time-ordered correlators. Submitted to *Physical Review Letters*. (LA-UR-20-22064)

Yan, B. and N. Sinitsyn. Analytical solution for a general quantum annealing problem. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-21-23292)

Yan, B. and W. H. Zurek. Convolution of decoherence: an interplay between Gaussian and exponential. Submitted to *Physical Review Letters*. (LA-UR-21-28440)

*Ying, S., S. Hayami and L. Shi-Zeng. Dimension transcendence and anomalous charge transport in magnets with moving multiple- spin textures. 2020. *Physical Review Research*. **2** (1): 013160. (LA-UR-19-23218 DOI: 10.1103/ PhysRevResearch.2.013160)

*Ying, S., S. Hayami and L. Shi-Zeng. Dimension transcendence and anomalous charge transport in magnets with moving multiple- spin textures. 2020. *Physical Review Research*. **2** (1): 013160. (LA-UR-19-25839 DOI: 10.1103/ PhysRevResearch.2.013160)

*Zegarac, A. and F. Caravelli. Memristive networks: From graph theory to statistical physics. 2019. *EPL (Europhysics Letters)*. **125** (1): 10001. (LA-UR-18-31372 DOI: 10.1209/0295-5075/125/10001)

*Zhang, Y., Y. Su and L. He. Local Berry Phase Signatures of Bilayer Graphene in Intervalley Quantum Interference.

2020. *Physical Review Letters*. **125** (11): 116804. (LA-UR-20-23249 DOI: 10.1103/PhysRevLett.125.116804)

*Zhentao, W., S. Ying, L. Shi-Zeng and C. D. Batista. Meron, skyrmion, and vortex crystals in centrosymmetric tetragonal magnets. 2021. *Physical Review B*. **103** (10): 104408. (LA-UR-20-29175 DOI: 10.1103/PhysRevB.103.104408)

*Zubatuk, T., B. T. Nebgen, N. E. Lubbers, J. S. Smith, R. Zubatuk, G. Zhou, C. F. Koh, K. M. Barros, O. Isayev and S. Tretiak. Machine learned H\xc3\xbcckel theory: Interfacing physics and deep neural networks. 2021. *The Journal of Chemical Physics*. **154** (24): 244108. (LA-UR-19-29765 DOI: 10.1063/5.0052857)

Conference Papers

Baertschi, A. and S. J. Eidenbenz. Deterministic Preparation of Dicke States. Presented at *22nd International Symposium on Fundamentals of Computation Theory*. (Copenhagen, Denmark, 2019-08-11 - 2019-08-14). (LA-UR-19-22718)

Baertschi, A. and S. J. Eidenbenz. Grover Mixers for QAOA: Shifting Complexity from Mixer Design to State Preparation. Presented at *IEEE International Conference on Quantum Computing and Engineering*. (Broomfield, Colorado, United States, 2020-10-12 - 2020-10-16). (LA-UR-20-23893)

Books/Chapters

Ghosh, D., M. J. Wolf, J. Kullgren and M. Pazoki. Characterising MAPbI 3 with the Aid of Electronic Structure Calculations. (LA-UR-19-27920)

Gifford, B. J. Functionalized Carbon Nanotube Excited States and Optical Properties. (LA-UR-19-23110)

Reports

Beckey, J. and A. Sone. Notes on QFI. Unpublished report. (LA-UR-20-28164)

S. Cerezo de la Roca, M. V. and P. J. Coles. Comment on "Characterizing the loss landscape of variational quantum circuits". Unpublished report. (LA-UR-20-26075)

Presentation Slides

Baertschi, A. Efficient Delivery with Mobile Agents. Presented at *CNLS Postdoc Seminar*, Los Alamos, New Mexico, United States, 2019-04-18 - 2019-04-18. (LA-UR-19-24756)

Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihal\xc3\xa1k. Near-gathering of energy-constrained mobile agents. Presented at *26th International Colloquium on Structural Information and Communication Complexity SIROCCO 2019*, L'Aquila, Italy, 2019-07-01 - 2019-07-04. (LA-UR-20-22307)

Baertschi, A. and S. J. Eidenbenz. Preparation and Compression of Symmetric Pure Quantum States. Presented at *ISTI*

Seminar (LANL), Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-20-22306)

Baertschi, A. and S. J. Eidenbenz. Deterministic Preparation of Dicke States. Presented at *22nd International Symposium on Fundamentals of Computation Theory FCT 2019*, Copenhagen, Denmark, 2019-08-11 - 2019-08-14. (LA-UR-20-22364)

Beckey, J. L., M. V. S. Cerezo de la Roca, P. J. Coles and A. Sone. Near-term Quantum Algorithm for Quantum Sensor Evaluation. . (LA-UR-21-21515)

Cen, J. Non-Hermitian Systems in Quantum Information. Presented at *CNLS External Advisory Committee (EAC) and Review*, Los Alamos, New Mexico, United States, 2021-05-14 - 2021-05-14. (LA-UR-21-24532)

Coker, A. A. Spin Dynamics in the Kagome Lattice. Presented at *2021 LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27684)

Garcia, A. E. CNLS Overview Presented to the CNLS External Advisory and LDRD Review Meeting. Presented at *CNLS Review Committee*, Los Alamos, New Mexico, United States, 2021-05-14 - 2021-05-14. (LA-UR-21-24607)

Ghosh, D. Halide Perovskite for Optoelectronics : Atomic-scale insights from ab initio Modeling. Presented at *MRS Fall Meeting*, Boston, Massachusetts, United States, 2019-12-02 - 2019-12-07. (LA-UR-19-32060)

Ghosh, D. Halide Perovskite for Optoelectronics: Atomic-scale Insights from ab initio Modeling. Presented at *Invited Talk at MRC, IISc, India*, Bangalore, India, 2020-01-22 - 2020-01-22. (LA-UR-20-20312)

Ghosh, D. Carrier Dynamics and Recombination in Low-Dimensional Halide Perovskites: Role of Structural Fluctuations. Presented at *APS March*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21858)

Ghosh, D. Charge Carrier Dynamics in Two-Dimensional Hybrid Perovskites: Impact of Spacer Cations. Presented at *NanoGe Fall Meeting*, Barcelona, Spain, 2020-10-20 - 2020-10-23. (LA-UR-20-28485)

Ghosh, D., A. J. Neukirch and S. Tretiak. Charge Carrier Dynamics in Two-Dimensional Hybrid Perovskites: Impact of Spacer Cations. Presented at *American Physical Society Meeting March 2021*, Denver, Colorado, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22459)

Gonzalez, D. G., G. Wang, E. R. Batista and P. Yang. Analysis of the thermodynamic stability of ThO2 and UO2 surfaces in the presence of surfactant ligands. . (LA-UR-20-24961)

Malla, R. K., A. B. Saxena and W. J. de Melo Kort-Kamp. Nonlinear planar Hall effect in graphene family monolayers. Presented at *APS March meeting, 2021*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22394)

S. Cerezo de la Roca, M. V. Talk: Trainability of Quantum Neural Network. . (LA-UR-20-24280)

S. Cerezo de la Roca, M. V. Science in 3. . (LA-UR-20-25832)

S. Cerezo de la Roca, M. V. Talk: Variational Quantum State Eigensolver. Presented at *QuAlg*, virtual, New Mexico, United States, 2020-09-22 - 2020-09-22. (LA-UR-20-27347)

Chacon Salazar, A. A. Ultrafast electron dynamics from atoms to solids. Presented at *Invited talk at the Asia Pacific Center for Theoretical Physics*, Pohang, Korea, South, 2019-05-11 - 2019-05-24. (LA-UR-19-24748)

Saxena, A. B. and J. Cen. Anti-PT-symmetric qubit: Decoherence and entanglement entropy. . (LA-UR-20-26139)

Smith, J. S., N. E. Lubbers, K. M. Barros, B. T. Nebgen, S. Tretiak, T. C. Germann, S. J. Fensin, A. E. Roitberg, O. Isayev, r. zubatyuk, L. Burakovsky, C. Devereux, K. Ranashingha, H. Suwa, C. Batista and G. Chern. Accelerated modeling of atomistic physics with machine learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-19 - 2019-02-21. (LA-UR-19-21274)

Smith, J. S., S. Tretiak, K. M. Barros, B. T. Nebgen, N. E. Lubbers, S. J. Fensin, T. C. Germann, O. Isayev, r. zubatyuk, A. Roitberg, C. Devereux, K. Ranashingha, H. Suwa, C. Batista and G. W. Chern. Accelerated Modeling of Atomistic Physics with Machine Learning. Presented at *American Chemical Society*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22830)

Smith, J. S., S. Tretiak, R. Zubatyuk, O. Isayev, A. E. Roitberg, B. T. Nebgen, N. E. Lubbers, S. J. Fensin, T. C. Germann and K. M. Barros. Machine learning of interatomic potentials. Presented at *Chesapeake Large-Scale Analytics Conference (CLSAC)*, Annapolis, Maryland, United States, 2019-10-07 - 2019-10-10. (LA-UR-19-30185)

Sone, A. Toward understanding work and heat in a quantum system. . (LA-UR-20-25924)

Sone, A. Precision sensing assisted by quantum-classical computation. . (LA-UR-20-27181)

Sone, A. Quantum Jarzynski Equality of Open Quantum Systems. Presented at *Invited talk by Centre for Quantum Dynamics at Griffith University*, Brisbane, Australia, 2020-10-20 - 2020-10-20. (LA-UR-20-28038)

Sone, A., M. V. S. Cerezo de la Roca, J. Beckey and P. J. Coles. Variational Quantum Algorithms for Estimating the Quantum Fisher Information. Presented at *Quantum Science Center, Quantum Algorithms Thrust meeting*, Oak Ridge, Tennessee, United States, 2020-10-28 - 2020-10-28. (LA-UR-20-28687)

Sone, A., Y. Liu and P. Cappellaro. Nonequilibrium work relations of open quantum systems in one-time measurement scheme \xc2\xa0. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21463)

Sone, A. and S. Deffner. Geometry of Thermal States – thermodynamics of quantum and classical coherence.

Presented at *March Meeting*, online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-21980)

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *Annual Conference on Magnetism and Magnetic Materials*, Las Vegas, Nevada, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31136)

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21986)

Su, Y. Twisted bilayer graphene: topological pumping and switching of topology by current. . (LA-UR-20-24896)

Subasi, Y. Quantum Algorithms For Noisy Intermediate-Scale Quantum Devices. . (LA-UR-18-31247)

Touil, A., B. Yan, D. Girolami, S. Deffner and W. H. Zurek. Eavesdropping on the Decohering Environment: Quantum Darwinism, Amplification, and the Origin of Objective Classical Reality. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21968)

Yan, B. The quantum zoo of butterflies. Presented at *Quantum Chao 2020 Seminars*, Albuquerque, New Mexico, United States, 2020-11-05 - 2020-11-05. (LA-UR-20-28711)

Yan, B. Information Scrambling in Complex Quantum Systems. . (LA-UR-21-24337)

Posters

Baertschi, A. and S. J. Eidenbenz. Deterministic Preparation of Dicke States with Applications to Symmetric Pure State Preparation and Quantum Compression. . (LA-UR-20-22305)

Cen, J. and A. B. Saxena. Joint Parity-Time and Anti-Parity-Time-symmetric Qubits. Presented at *IEEE QUANTUM WEEK*, Broomfield, Colorado, United States, 2021-10-18 - 2021-10-18. (LA-UR-21-27922)

Ghosh, D., A. J. Neukirch and S. Tretiak. Hybrid Perovskites for Solar Cells: Atomic-Scale Insights into Local Structure, Defects and Charge Dynamics. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28619)

Ghosh, D., A. J. Neukirch and S. Tretiak. Charge Carrier Dynamics in Two-Dimensional Hybrid Perovskites: Impact of Spacer Cations. Presented at *CINT Annual Meeting (Virtual), LANL*, Los Alamos, New Mexico, United States, 2020-09-21 - 2020-09-23. (LA-UR-20-27244)

S. Cerezo de la Roca, M. V., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation (VQFE). . (LA-UR-19-28193)

S. Cerezo de la Roca, M. V., L. Cincio and P. J. Coles. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states Or, how to compare two quantum states on a quantum computer. . (LA-UR-19-24875)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, T. C. Germann, S. J. Fensin and K. M. Barros. Discovering physics from disorder: active learning a robust potential for aluminum. . (LA-UR-19-32169)

Smith, J. S., K. M. Barros, S. Tretiak, N. Mathew, N. E. Lubbers and B. T. Nebgen. Atomistic Potentials for molecules and materials from machine learning. . (LA-UR-19-24846)

Sone, A., J. Beckey, M. V. S. Cerezo de la Roca and P. J. Coles. Quantum Fisher information estimation via hybrid quantum-classical computation. Presented at *Quantum Techniques in Machine Learning 2020*, Cambridge, Massachusetts, United States, 2020-11-09 - 2020-11-12. (LA-UR-20-28727)

Su, Y. and S. Lin. Switching of Valley Polarization by Electric Current in Twisted Bilayer Graphene. Presented at *2020 Theory Winter School: Quantum Matter Without Quasiparticles*, Tallahassee, Florida, United States, 2020-01-06 - 2020-01-10. (LA-UR-20-20140)

Weight, B. M., B. J. Gifford and S. Tretiak. Interacting Pairs of Surface Defects on Carbon Nanotubes. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27817)

Yan, B. and N. Sinitsyn. Information scrambling and the anti butterfly effect. Presented at *APS March Meeting 2021*, Nashville, Tennessee, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-20815)

Theoretical and Experimental Materials Science

Filip Ronning
20190497CR-IMS

Project Description

The national security mission of Los Alamos National Lab will require new materials solutions to solve the problems that will arise in tomorrow's challenges. High risk/high reward ideas that can be quickly and efficiently explored are needed to identify opportunities for new growth areas. This project will pursue such projects within theoretical and experimental material science.

Technical Outcomes

The Institute for Materials Science under the National Security Education Center at Los Alamos National Laboratory identified and funded priority research on materials informatics, machine learning, advanced manufacturing, and materials for quantum information. Our program provided an agile response to capitalize on opportunities quickly, provide funding where it is occasionally constrained, provide training opportunities for new staff, and develop new capabilities in the area of materials science central to our mission and materials strategy.

Publications

Journal Articles

Bacak, M., J. Valsecchi, J. Capek, E. Polatidis, A. Kaestner, A. Arabi-Hashemi, I. I. Kruk, C. Leinenbach, A. M. Long, A. S. Tremsin, S. C. Vogel, E. B. Watkins and M. Strobl. Neutron dark-field imaging applied to porosity and deformation-induced phase transitions in additively manufactured steels. Submitted to *Materials & Design*. (LA-UR-20-25975)

Blaschke, D. A general solution for accelerating screw dislocations in arbitrary slip systems with reflection symmetry. Submitted to *Journal of the Mechanics and Physics of Solids*. (LA-UR-20-25951)

Blaschke, D., J. Chen, S. J. Fensin and B. A. Szajewski. Clarifying the definition of 'transonic' screw dislocations. Submitted to *Philosophical Magazine*. (LA-UR-20-25514)

Blaschke, D., J. Chen, S. J. Fensin and B. A. Szajewski. Clarifying the definition of 'transonic' screw dislocations. Submitted to *Philosophical Magazine*. (LA-UR-20-25514)

Brounstein, Z. R., C. M. Yeager and A. Labouriau. Development of New Formulations of Biocompatible Green Resins for Additive Manufacturing. Submitted to *Polymer*. (LA-UR-20-30333)

Brounstein, Z. R., C. M. Yeager and A. Labouriau. Development of Antimicrobial PLA Composites for Fused Filament Fabrication. Submitted to *Polymers*. (LA-UR-21-20929)

*Brounstein, Z., S. Talley, J. H. Dumont, J. Zhao, K. Lee and A. Labouriau. Fused filament fabrication of polymer composites for extreme environments. 2020. *Journal of Materials Research*. **35** (12): 1493-1503. (LA-UR-20-21484 DOI: 10.1557/jmr.2020.118)

Caravelli, F., F. Andrade and A. Halbritter. Modeling quantum transport on a few atoms filament. Submitted to *Physical Review A*. (LA-UR-21-29021)

*Enriquez, E. M., Q. Li, P. R. Bowlan, P. Lu, B. Zhang, L. Li, H. Wang, A. J. Taylor, D. A. Yarotski, R. P. Prasankumar, S. V. Kalinin, Q. Jia and A. Chen. Induced ferroelectric phases in SrTiO by a nanocomposite approach. 2020. *Nanoscale*. **12** (35): 18193-18199. (LA-UR-20-24150 DOI: 10.1039/D0NR03460F)

Pandey, A., J. G. Gigax and R. Pokharel. Machine learning force-field to develop and optimize multi-components alloys. Submitted to *Computational Materials Science*. (LA-UR-22-20252)

H. A. *. B. I. J. *. L. R. A. *. D. K. *. M. E. Peng, X. *., A. Hunter, R. A. Lebensohn and X. Peng. Non-orthogonal computational grids for studying dislocation motion in phase field approaches. 2021. *Computational Materials Science*. **200**: 110834. (LA-UR-21-25715 DOI: 10.1016/j.commatsci.2021.110834)

*Pettes, M. T., A. Londono Calderon, D. J. Williams, B. H. Savitzky, C. Ophus, S. Ma, H. Zhu and M. M. Schneider. Intrinsic helical twist and chirality in ultrathin tellurium nanowires. 2021. *Nanoscale*. **13** (21): 9606-9614. (LA-UR-21-21904 DOI: 10.1039/D1NR01442K)

*Pettes, M. T., A. Londono Calderon, D. J. Williams, C. Ophus, B. Savitsky and M. M. Schneider. Local Lattice Deformation of Tellurene Grain Boundaries by Four-Dimensional Electron Microscopy. 2021. *The Journal of Physical Chemistry C*. **125** (6): 3396-3405. (LA-UR-20-27603 DOI: 10.1021/acs.jpcc.1c00308)

Pettes, M. T., A. Londono Calderon, R. Dhall, C. Ophus, Y. Wang, E. Dervishi-Whetham, H. S. Kang, C. Lee and J. Yoo. Visualizing Grain Statistics in MOCVD WSe through Four-Dimensional Scanning Transmission Electron Microscopy. 2022. *Nano Letters*. (LA-UR-21-30267 DOI: 10.1021/acs.nanolett.1c04315)

*Reichhardt, C. and C. J. O. Reichhardt. Collective effects and pattern formation for directional locking of disks moving through obstacle arrays. 2020. *Physical Review E*. **102** (2): 022608. (LA-UR-20-24219 DOI: 10.1103/PhysRevE.102.022608)

Reichhardt, C. and C. J. Reichhardt. Directional locking effects for active matter particles coupled to a periodic substate. Submitted to *Physical Review E*. (LA-UR-20-26211)

Reichhardt, C. and C. J. Reichhardt. Directional Clogging and Phase Separation for Particle Flow Through Peridoic and Diluted Obstacle Arrays. Submitted to *Soft Matter*. (LA-UR-20-27479)

Reichhardt, C. and C. J. Reichhardt. Active Matter Commensuration and Frustration Effects on Periodic Substrates. Submitted to *Physical Review Letters*. (LA-UR-20-28967)

Scheinker, A. and R. Pokharel. Adaptive 3D convolutional neural network-based reconstruction method for 3D coherent diffraction imaging. Submitted to *Journal of Applied Physics*. (LA-UR-20-24185)

Sirica, N. S., H. Hedayat, D. Bungini, M. Koehler, L. Li, D. Parker, D. Mandrus, C. Dallera, E. Carpene and N. Mannella. Disentangling electronic, lattice, and spin dynamics in the chiral helimagnet Cr1/3NbS2. 2021. *Physical Review B*. **104** (17): 174426. (LA-UR-21-28094 DOI: 10.1103/PhysRevB.104.174426)

*Su, Y. and S. Lin. Current-Induced Reversal of Anomalous Hall Conductance in Twisted Bilayer Graphene. 2020. *Physical Review Letters*. **125** (22): 226401. (LA-UR-20-21206 DOI: 10.1103/PhysRevLett.125.226401)

*C. Tan, A. K., P. Ho, J. Lourembam, L. Huang, H. K. Tan, C. J. O. Reichhardt, C. Reichhardt and A. Soumyanarayanan. Visualizing the strongly reshaped skyrmion Hall effect in multilayer wire devices. 2021. *Nature Communications*. **12** (1): 4252. (LA-UR-20-24857 DOI: 10.1038/s41467-021-24114-8)

*Vizarim, N. P., C. Reichhardt, P. A. Venegas and C. J. O. Reichhardt. Guided skyrmion motion along pinning array interfaces. 2021. *Journal of Magnetism and Magnetic Materials*. **528**: 167710. (LA-UR-20-26712 DOI: 10.1016/j.jmmm.2020.167710)

Zhang, J., L. Wang, J. Zhu and Y. Zhao. Structural Disorder, Sublattice Melting and Thermo-Elastic Properties of Anti-Perovskite Li3OBr under High Pressure and Temperature. Submitted to *Applied Physics Letters*. (LA-UR-20-23865)

Conference Papers

Martinez, B., M. F. Silva, H. Jung, A. W. Green, K. E. Coombs, P. Nath, J. F. Harris and D. D. L. Mascarenas. An Unsupervised Machine Learning Technique for Detecting Cardiac Arrhythmia From Video of Cardiac Myocytes. Presented at *Visual Recognition for Medical Images*. (Seoul, Korea, South, 2019-10-27 - 2019-10-27). (LA-UR-19-27699)

Reports

Blaschke, D. Towards predicting material strength under extreme conditions: Summary Report for the IMS Rapid Response 2020-R&D-1 project. Unpublished report. (LA-UR-20-26987)

Eftink, B. P., T. R. Jacobs and T. J. I. Ulrich. Internal friction measurements for measuring DBTT in reactor relevant alloys. Unpublished report. (LA-UR-19-30068)

Firestone, M. A. and P. M. J. Welch. Predictive topology optimization for 4D printed soft materials. Unpublished report. (LA-UR-20-27703)

Hunter, A. and E. Martinez Saez. Integrating Kinetic Monte Carlo and the Phase Field Dislocation Dynamics to account for thermally activated plasticity Final Report. Unpublished report. (LA-UR-20-27718)

Kim, H., J. G. Gigax, S. A. Maloy and O. El Atwani. Development of high performance high-entropy alloys and evaluation of radiation response under stress. Unpublished report. (LA-UR-21-29560)

Kiplinger, J. L., B. P. Nolen and J. K. Pagano. Transforming the Uranium Fuel Cycle: Safe & Economical Conversion of DUF6 to DUF4. Unpublished report. (LA-UR-19-29815)

Lawrence, S. K., A. Llobet Megias and M. S. Freeman. Uranium Hydride Experiment Capability Development at pRad. Unpublished report. (LA-UR-19-29700)

Lee, K. Development of 3D Printable Conductive Wires for Flexible Electronics. Unpublished report. (LA-UR-21-29842)

Li, N. Summary Report for Institute for Materials Science Rapid Response Project: Dual Phase High Entropy Alloys with Unprecedented Irradiation Tolerance. Unpublished report. (LA-UR-21-29902)

Lin, S. Report for the project "Control valley polarization in two dimensional materials by electric current". Unpublished report. (LA-UR-20-27807)

Morales, D. P., J. M. Kelliher, T. Elkin and J. H. Werner. Bioprospecting: Nanoscale Recognition in a Mesoscale Material. Unpublished report. (LA-UR-19-29845)

Pandey, A. Project Summary:Adaptive machine-learned force field development for high entropy alloy studies.. Unpublished report. (LA-UR-21-29588)

Pettes, M. T., M. M. Schneider, M. T. Janish and A. Londono Calderon. IMS Rapid Response FY21 Summary Report for: Integrating Patterned Probes with Four-Dimensional Scanning Transmission Electron Microscopy for Unrivaled

Crystallographic Structure Determination in Nanomaterials. Unpublished report. (LA-UR-21-29955)

Pokharel, R. and A. Scheinker. Adaptive Machine Learning for Bragg Coherent Diffraction Imaging (BCDI) of 3D Electron Density Maps with Application to La2-xBaxCuO4 (LBCO) High Temperature Superconductor Studies. Unpublished report. (LA-UR-20-27678)

Reichhardt, C. J. Artificial Intelligence for Dynamic Phase Transitions in Materials. Unpublished report. (LA-UR-20-27740)

Scott, B. L., A. P. Shivprasad and J. T. White. Defining Phase Diagrams in Accident Tolerant Fuels. Unpublished report. (LA-UR-19-31173)

Thomas, S. M. Report: The origin of nematicity in 4f materials revealed by three-axis dilatometry. Unpublished report. (LA-UR-20-27838)

Vogel, S. C., A. M. Long, E. B. Watkins and E. N. Caspi. Summary report for "Neutron Phase Contrast Imaging for <1micrometer Feature Detection in Bulk Materials". Unpublished report. (LA-UR-19-30103)

Vogel, S. C. and E. B. Watkins. Neutron Imaging Using Grating Interferometry: Exploiting phase contrast and dark-field imaging for <1\xce\xbcm feature detection in bulk materials. Unpublished report. (LA-UR-20-27576)

White, A. J. Capability development for the ab-initio calculation of material properties at any temperature.. Unpublished report. (LA-UR-20-27726)

Zhang, J. Project Report for "Lithium-Rich Electrolytes for All Solid-State, All Spinel Ion Batteries". Unpublished report. (LA-UR-20-27893)

Presentation Slides

Blaschke, D. Towards predicting material strength under extreme conditions. . (LA-UR-20-27230)

Brounstein, Z. R. Developing filament feedstock of polymer composites for additive manufacturing. Presented at *Virtual Student Symposium 2020*, Los Alamos, New Mexico, United States, 2020-08-20 - 2020-08-21. (LA-UR-20-25720)

Brounstein, Z. R. Thermoplastics and Thermosets: Multifunctionality, 3D printing, and Accelerated Aging_v4. . (LA-UR-20-28966)

Brounstein, Z. R. Thermoplastics and Thermosets Multifunctionality, 3D printing, and Accelerated Aging. . (LA-UR-20-29035)

Londono Calderon, A., D. J. Williams, B. H. Savitzky, C. Ophus, S. Ma, H. Zhu, M. M. Schneider and M. T. Pettes. Intrinsic Helical Twist and Chirality in Ultrathin Tellurium Nanowires. Presented at *2021 Microscopy & Microanalysis*, Pittsburgh, Pennsylvania, United States, 2021-08-01 - 2021-08-05. (LA-UR-21-21748)

Chen, A. Composition gradient thin films: A new way to explore high-throughput film synthesis in complex oxides. . (LA-UR-19-30132)

Eftink, B. P., T. J. I. Ulrich, T. R. Jacobs, J. G. Gigax, O. Anderoglu, T. A. Saleh and S. A. Maloy. Internal friction measurements for measuring DBTT in reactor relevant alloys. Presented at *IMS 2019 presentations*, Los Alamos, New Mexico, United States, 2019-10-09 - 2019-10-09. (LA-UR-19-30070)

Firestone, M. A. and P. M. J. Welch. Predictive topology optimization for 4D printed soft materials. Presented at *IMS Rapid Response Roundup 2020*, Los Alamos, New Mexico, United States, 2020-10-06 - 2020-10-06. (LA-UR-20-27780)

Gigax, J. G., H. Kim, S. A. Maloy and O. El Atwani. Development of high performance high-entropy alloys and evaluation of radiation response under stress. . (LA-UR-21-29849)

Greer, S. M. and B. Stein. Developing A Broadband Low-Frequency Electron Paramagnetic Resonance Spectrometer. Presented at *IMS Rapid Response Roundup Alternative*, Los Alamos, New Mexico, United States, 2021-09-29 - 2021-09-29. (LA-UR-21-29595)

Huber, R. C., E. B. Watkins, B. D. Bartram, D. M. Dattelbaum, L. L. Gibson, R. L. Gustavsen and J. L. Jordan. X-ray Diffraction and Scattering to Probe Structural Changes During Dynamic Compression of Polymers. Presented at *Carbon in Extremes*, Santa Fe, New Mexico, United States, 2019-10-28 - 2019-10-28. (LA-UR-19-30899)

Huber, R. C., E. B. Watkins and D. M. Dattelbaum. Small Angle X-ray Scattering Diagnostic Pair to Gas Gun. . (LA-UR-19-29956)

Hunter, A. and E. Martinez Saez. Integrating Kinetic Monte Carlo and Phase Field Dislocation Dynamics to account for thermally activated plasticity. . (LA-UR-20-27770)

Kim, H., J. G. Gigax, S. A. Maloy, M. R. Chancey, O. El Atwani and N. Li. Development of high performance high-entropy alloys and evaluation of radiation response under stress. Presented at *TMS 2nd world congress on HEA 2021*, Charlotte, North Carolina, United States, 2021-12-06 - 2021-12-08. (LA-UR-22-21421)

Kim, H., J. G. Gigax, S. A. Maloy and O. El Atwani. Development of high performance high-entropy alloys and evaluation of radiation response under stress. . (LA-UR-21-29895)

Kiplinger, J. L. Transforming the Uranium Fuel Cycle: Safe & Economical Conversion of DUF6 to DUF4. . (LA-UR-19-30142)

Lawrence, S. K., A. Llobet Megias and M. S. Freeman. Uranium Hydride Experiment Capability Development at pRad. Presented at *2019 IMS Rapid Response Roundup*, Los Alamos, New Mexico, United States, 2019-10-09 - 2019-10-09. (LA-UR-19-30117)

Lee, K. Development of 3D printable conductive wires for flexible electronics. Presented at *IMS Rapid Response*

Roundup 2021, Los Alamos, New Mexico, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-29843)

Li, N., D. Chen, Y. Chen, J. Weaver, Y. Wang, S. J. Fensin, S. A. Maloy and A. Misra. Heavy Ion Irradiation Response of FeCrNiMn and FeCrNiMnAl High Entropy Alloys. Presented at *TMS 2021 Annual Meeting*, Los Alamos, New Mexico, United States, 2021-03-15 - 2021-03-18. (LA-UR-21-22549)

Lin, S. Control valley polarization in two dimensional materials by electric current. . (LA-UR-20-27840)

Minko, Y. Stimuli-responsive Materials for the Colorimetric Detection of CWAs and Novichok agents. Presented at *Institute for Materials Science Los Alamos Rapid Response Roundup 2021*, Los Alamos, New Mexico, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-29412)

Morales, D. P., J. H. Werner, P. S. G. Chain, J. M. Kelliher, T. Elkin and P. Nath. Bioprospecting: Nanoscale recognition in a mesoscale material. . (LA-UR-19-30076)

Morgan, R. V., K. T. Pittman, R. K. Walzel, A. F. Tirado, A. N. Marchi, M. R. Middlemas and J. D. Bernardin. The Production of Complex Lightweight Radiation Shield Materials Using Additive Manufacturing Technologies. Presented at *IMS Rapid Response Roundup 2019*, Los Alamos, New Mexico, United States, 2019-10-09 - 2019-10-09. (LA-UR-19-31304)

Pandey, A. Physics-informed data-driven surrogate modeling for advancing experiments and the study of novel materials. . (LA-UR-21-27990)

Peng, X. Computational Methods for Structure-Property Relations in Heterogeneous Materials. . (LA-UR-21-22172)

Reichhardt, C. J. Artificial Intelligence for Dynamic Phase Transitions in Materials. . (LA-UR-20-27900)

Scheinker, A. and R. Pokharel. Adaptive Machine Learning for Bragg Coherent Diffraction Imaging (BCDI) of 3D Electron Density Maps with Application to La2-xBaxCuO4 (LBCO) High Temperature Superconductor Studies. . (LA-UR-20-27907)

Scheinker, A. and R. Pokharel. Adaptive Machine Learning for 3D Bragg Coherent Diffraction Imaging Reconstructions. Presented at *TMS 2021*, Orlando, Florida, United States, 2021-03-22 - 2021-03-22. (LA-UR-21-23604)

Scott, B. L., J. T. White, A. P. Shivprasad and J. R. Wermer. Defining Phase Diagrams in Accident Tolerant Fuels. . (LA-UR-19-30107)

Sirica, N. S. Resolving the Spinon Continuum. . (LA-UR-21-29850)

Thomas, S. M. The origin of nematicity in 4f materials revealed by three-axis dilatometry. Presented at *Rapid Response Roundup 2020*, Los Alamos, New Mexico, United States, 2020-10-06 - 2020-10-06. (LA-UR-20-27839)

Vogel, S. C., E. B. Watkins and A. M. Long. Neutron Phase Contrast Imaging for <1 micrometer Feature Detection in Bulk Materials. . (LA-UR-19-30224)

Vogel, S. C., M. Roth, A. S. Losko, D. C. Gautier, K. L. Knickerbocker, J. C. Fernandez, A. Kleinschmidt, K. F. Schoenberg, N. Mitura, J. F. Hunter and R. O. Nelson. Short-pulse Laser-driven Moderated Neutron Source. Presented at *1st Experts Meeting on Fast Neutron Imaging*, Munich, Germany, 2019-10-21 - 2019-10-23. (LA-UR-19-30196)

White, A. J. Capability development for the ab-initio calculation of material properties at any temperature. . (LA-UR-20-27825)

White, A. J. Density Functional Theory for Matter in Extreme Conditions: Warm Dense Matter to Hot Dense Plasmas. . (LA-UR-20-28177)

White, A. J. Density Functional Theory for Warm Dense Matter and Hot Dense Plasmas: from EOS to stopping power. Presented at *University of Rochester / LLE Seminar*, Virtual, New Mexico, United States, 2021-04-07 - 2021-04-07. (LA-UR-21-23245)

Other

L. Mascarenas, D. D., B. Martinez, K. E. Coombs, A. W. Green, P. Nath and J. F. Harris. An Unsupervised Machine Learning Technique for Characterizing the Electro-Mechanical Dynamics of Heart Cells from Calcium Imaging Video. Audio/Visual. (LA-UR-19-30169)

Nuclear and Particle Futures

The Neutron Electric Dipole Moment as a Gateway to New Physics

Takeyasu Ito
20190041DR

Project Description

The research supported by this project addresses the question "Why does the Universe that we live in have so much more matter than antimatter", one of the biggest questions in present day science. This project, on completion, will have demonstrated a capability to perform next generation experiments looking for neutron electric dipole moment, have controlled systematics important for all such experiments, and have developed a theory to use results from these experiments to constrain theories of new physics. Collectively, this research will have a profound impact on our understanding of the interaction among the fundamental building blocks of our world and the history of the Universe. The methods of precision measurements and computation will benefit other researches performed at the Laboratory and elsewhere. The theory employs the tools of Lattice Quantum ChromoDynamics, which have consistently driven the development of novel computer architectures for a long time. The theoretical work done as part of this project will not only enhance the laboratory's stature among theoretical physicists, thus benefiting in hire and retention of personnel, but will also develop and maintain the capability of employing high performance computing architectures in service of simulating challenging scientific problems.

Publications

Journal Articles

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti and B. Yoon. Contribution of the QCD \xce\x98-term to neutron electric dipole moment. Submitted to *Physical Review D*. (LA-UR-20-30515)

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti and B. Yoon. Quark Chromo-Electric Dipole Moment Operator on the Lattice. Submitted to *Physical Review D*. (LA-UR-21-21913)

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti and B. Yoon. Contribution of the gluon chromo-EDM to nucleon electric dipole moment. Submitted to *Physical Review D*. (LA-UR-21-22073)

*Cirigliano, V., A. Crivellin, W. Dekens, J. de Vries, M. Hoferichter and E. Mereghetti. Violation in Higgs-Gauge Interactions: From Tabletop Experiments to the LHC. 2019. *Physical Review Letters*. **123** (5): 051801. (LA-UR-19-22027 DOI: 10.1103/PhysRevLett.123.051801)

*Cirigliano, V., E. Mereghetti and P. Stoffer. Non-perturbative renormalization scheme for the C P -odd three-gluon operator. 2020. *Journal of High Energy Physics*. **2020** (9): 94. (LA-UR-20-20500 DOI: 10.1007/JHEP09(2020)094)

*Gupta, R., B. joo, T. Bhattacharya, S. Park, B. Yoon, S. Mondal and F. Winter. Nucleon momentum fraction, helicity and transversity from 2+1-flavor lattice QCD. 2021. *Journal of High Energy Physics*. **2021** (4): 44. (LA-UR-20-28586 DOI: 10.1007/JHEP04(2021)044)

Gupta, R., M. Hoferichter, E. Mereghetti, B. Yoon, T. Bhattacharya and S. Park. The nucleon sigma term from lattice QCD. Submitted to *Physical Review Letters*. (LA-UR-21-24759)

Gupta, R., b. Joo, T. Bhattacharya, B. Yoon, S. Park, S. Mondal, F. winter and Y. C. Jang. Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD. Submitted to *Physical Review D*. (LA-UR-21-20526)

Jang, Y. C., T. Bhattacharya, R. Gupta, H. W. Lin and B. Yoon. Updates on Nucleon Form Factors from Clover-on-HISQ Lattice Formulation. *PoS - Proceedings of Science*. (LA-UR-19-20696 DOI: 10.22323/1.334.0123)

Mereghetti, E., C. Monahan, M. Rizik, A. Shindler and P. Stoffer. One loop matching for quark dipole operators in the gradient flow scheme. Submitted to *Journal of High Energy Physics*. (LA-UR-21-31507)

Mereghetti, E., J. de Vries, E. Epelbaum, L. Girlanda, A. Gnech and M. Viviani. Parity- and time-reversal-violating nuclear forces. Submitted to *Frontiers in Physics*. (LA-UR-20-20558)

Mereghetti, E., L. Platter, Z. Yang, J. Vanasse and M. Schindler. Electric dipole moments of three-nucleon systems in pionless EFT. Submitted to *Physical Review C*. (LA-UR-20-28735)

*T. Nguyen, N. T., G. T. Kenyon and B. Yoon. A regression algorithm for accelerated lattice QCD that exploits sparse inference on the D-Wave quantum annealer. 2020. *Scientific Reports*. **10** (1): 10915. (LA-UR-19-31717 DOI: 10.1038/s41598-020-67769-x)

Yoon, B., C. C. Chang, G. Kenyon, N. T. T. Nguyen-Fotiadis and E. Rrapaj. Prediction and compression of lattice QCD data using machine learning algorithms on quantum annealer. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-31665)

Yoon, B., T. Bhattacharya, V. Cirigliano and R. Gupta. Neutron Electric Dipole Moments with Clover Fermions. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-32467 DOI: 10.22323/1.363.0243)

Zhang, R., H. Lin and B. Yoon. Probing nucleon strange and charm distributions with lattice QCD. Submitted to *arXiv*. (LA-UR-20-23850)

*Zhang, R., Z. Fan, R. Li, H. Lin and B. Yoon. Machine-learning prediction for quasiparton distribution function matrix elements. 2020. *Physical Review D*. **101** (3): 034516. (LA-UR-19-30235 DOI: 10.1103/PhysRevD.101.034516)

Conference Papers

Bhattacharya, T., B. Yoon, R. Gupta and V. Cirigliano. Neutron Electric Dipole Moment from Beyond the Standard Model. Presented at *The 36th Annual International Symposium on Lattice Field Theory - LATTICE2018*. (East Lansing, Michigan, United States, 2018-07-22 - 2018-07-28). (LA-UR-18-31631)

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti and B. Yoon. Calculation of neutron electric dipole moment due to the QCD topological term, Weinberg three-gluon operator and the quark chromoelectric moment. Presented at *The 38th International Symposium on Lattice Field Theory*. (Boston, Massachusetts, United States, 2021-07-26 - 2021-07-26). (LA-UR-21-31575)

Gupta, R., M. Hoferichter, T. Bhattacharya, E. Mereghetti, B. Yoon and S. Park. The pion-nucleon sigma term from Lattice QCD. Presented at *The 10th International Workshop on Chiral Dynamics*. (Beijing, China, 2021-11-15 - 2021-11-19). (LA-UR-22-22580)

Gupta, R., M. Hoferichter, T. Bhattacharya, V. Cirigliano, E. Mereghetti, Y. C. Jang, B. Joo, F. Winter, B. Yoon, S. Park and S. Mondal. Excited states and precision results for nucleon charges and form factor. Presented at *The 38th International Symposium on Lattice Field Theory, LATTICE2021 26th-30th July, 2021 Zoom/ Gather@Massachusetts Institute of Technology*. (Cambridge, Massachusetts, United States, 2021-07-26 - 2021-07-30). (LA-UR-21-32449)

Park, S., T. Bhattacharya, R. Gupta, B. Yoon, Y. C. Jang, H. W. Lin, K. Orginos, D. Richards and B. Joo. Nucleon Charges and Form Factors using Clover Fermions. Presented at *the 37th international conference on lattice field theory*. (Wuhan, China, 2019-06-16 - 2019-06-22). (LA-UR-19-31873)

Reports

Bhattacharya, T., T. Blum, V. Cirigliano, J. de Vries, D. P. DeMille, N. R. Hutzler, T. Ito, C. Liu, W. M. Morse, M. Reece and P. Winter. Elecric dipole moments and the search for new physics. Unpublished report. (LA-UR-22-22083)

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti, B. Yoon, W. G. Dekens, J. de Vries, A. Shindler and C. Monahan. Constraining Physics Beyond the Standard Model using Electric Dipole Moments. Unpublished report. (LA-UR-20-26774)

Burdine, J. F. and T. Ito. Photographs of the magnetically shielded room being assembled in Area B, Batch 2. Unpublished report. (LA-UR-21-24986)

Burdine, J. F. and T. Ito. Photographs of the magnetically shielded room being assembled in Area B, Batch 3. Unpublished report. (LA-UR-21-25641)

Burdine, J. F. and T. Ito. Photographs of the magnetically shielded room being assembled in Area B, Batch 4. Unpublished report. (LA-UR-21-25815)

Burdine, J. F. and T. Ito. Photographs of the magnetically shielded room being assembled in Area B, Batch 6. Unpublished report. (LA-UR-22-20578)

Cirigliano, V., T. Bhattacharya, Z. Davoudi, T. Izubuchi, P. Shanahan, M. Wagman and S. Syritsin. The Role of Lattice QCD in Searches for Violations of Fundamental Symmetries and Signals for New Physics. Unpublished report. (LA-UR-19-22184)

Gupta, R., T. Bhattacharya, V. Cirigliano, E. Mereghetti, B. Yoon, S. Mondal, S. Park, S. Alioli, R. Boughezal, Y. Jang, H. W. Lin, S. Pastore, F. Petriello and A. Young. Probing Scalar and Tensor Interactions at the TeV Scale. Unpublished report. (LA-UR-20-26760)

Park, S. Note: NPR of bilinears on N_f=2+1 QCD. Unpublished report. (LA-UR-21-22575)

Presentation Slides

Bhattacharya, T. nEDM Theory. Presented at *Workshop on Fundamental Physics at the Second Target Station (FPSTS19)*, Oak Ridge, Tennessee, United States, 2019-07-26 - 2019-07-27. (LA-UR-19-27343)

Bhattacharya, T. Gradient Flow. Presented at *Workshop on Lattice QCD*, Santa Fe, New Mexico, United States, 2019-08-26 - 2019-08-30. (LA-UR-19-28608)

Bhattacharya, T. Neutron Electric Dipole Moments. Presented at *Workshop on Lattice QCD*, Santa Fe, New Mexico, United States, 2019-08-26 - 2019-08-30. (LA-UR-19-28747)

Bhattacharya, T. Neutron Electric Dipole Moment & QFT on quantum computers. . (LA-UR-20-22412)

Bhattacharya, T. Neutron Electric Dipole Moment. . (LA-UR-20-22758)

Bhattacharya, T. Nucleon Matrix Elements for HEP and NP. . (LA-UR-20-26716)

Bhattacharya, T. Lattice Gauge Theory for High Energy Physics: Fundamental Symmetries brief. Presented at *Snowmass 2021 Community Planning Meeting*, Online, Illinois, United States, 2020-10-05 - 2020-10-07. (LA-UR-20-27911)

Bhattacharya, T. Calculating neutron properties to look for new physics. . (LA-UR-21-22554)

Bhattacharya, T. Neutron Electric Dipole Moment. . (LA-UR-21-23965)

Bhattacharya, T. Neutron Electric Dipole Moment and Field Theory on Quantum Devices. . (LA-UR-21-25854)

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti and B. Yoon. Lattice QCD calculation of neutron EDM induced by QCD $\\theta$-term and quark chromo-EDM. Presented at *Beyond-the-Standard-Model Physics with Nucleons and Nuclei*, Online, New Mexico, United States, 2020-07-22 - 2020-07-22. (LA-UR-20-29522)

Bhattacharya, T., V. Cirigliano, R. Gupta, E. Mereghetti and B. Yoon. Calculation of neutron electric dipole moment due to the QCD topological term, Weinberg three-gluon operator and the quark chromoelectric moment. Presented at *The 38th international Symposium on Lattice Field Theory*, Boston, Massachusetts, United States, 2021-07-26 - 2021-07-30. (LA-UR-21-27233)

Gupta, R. Probing novel phenomena with protons and neutrons using Lattice QCD at LANL:. . (LA-UR-20-22643)

Gupta, R. Unitarity of CKM Matrix: |Vud| from neutron decay. Presented at *Snowmass RF02 Topical group*, Virtual, New Mexico, United States, 2020-10-02 - 2020-10-02. (LA-UR-21-20528)

Gupta, R. Lattice QCD at LANL (2020 PR). . (LA-UR-21-22424)

Gupta, R. Overview of HEP Theory and QuantISED Efforts and Nucleon Matrix elements. Presented at *DOE HEP Review*, Virtual, New Mexico, United States, 2021-07-06 - 2021-07-08. (LA-CP-21-20598)

Gupta, R. Excited states and precision results for nucleon charges and form factors. Presented at *38 International Symposium on Lattice Field Theory, 2021*, Boston (virtual), Massachusetts, United States, 2021-07-26 - 2021-07-26. (LA-UR-21-27234)

Gupta, R., H. Lin, B. Yoon, S. Mondal, T. Bhattacharya and S. Park. Flavor diagonal matrix elements. Presented at *USQCD all hands meeting*, Boston (virtual), Massachusetts, United States, 2021-04-30 - 2021-04-30. (LA-UR-21-24214)

Gupta, R., M. Hoferichter, E. Mereghetti, T. Bhattacharya, B. Yoon and S. Park. The pion–nucleon sigma term from lattice QCD. Presented at *Chiral Dynamics 2021*, Beijing, China, 2021-11-15 - 2021-11-15. (LA-UR-21-31181)

Gupta, R., S. Iyer and A. J. Taylor. LANL HEP Strategic Overview and FY23 Budget Planning. Presented at *DOE Budget Brief*, Los ALamos, New Mexico, United States, 2021-06-09 - 2021-06-09. (LA-UR-21-25516)

Hassan, M. T. The Current Status of the LANL nEDM Experiment. Presented at *APS April Meeting*, Washington D.C., District Of Columbia, United States, 2020-04-18 - 2020-04-18. (LA-UR-20-23006)

Hassan, M. T. TRIUMF Guide Tests Photos. . (LA-UR-20-30434)

Hassan, M. T. Development of a New Neutron Electric Dipole Moment Experiment at LANL. . (LA-UR-21-28058)

Ito, T. A New Experiment to Search for the Neutron's Electric Dipole Moment at LANSCE. Presented at *LANSCE Users' Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-07. (LA-UR-18-30605)

Ito, T. nEDM Experiment at Los Alamos National Laboratory. Presented at *Workshop on "Particle Physics with Neutrons at the ESS"*, Stockholm, Sweden, 2018-12-10 - 2018-12-14. (LA-UR-18-31385)

Ito, T. nEDM — North American Efforts. Presented at *ACFI Workshop on "Theoretical Issues and Experimental Opportunities in Searches for Time Reversal Invariance Violation Using Neutrons"*, Amherst, Massachusetts, United States, 2018-12-06 - 2018-12-08. (LA-UR-18-31384)

Ito, T. LANL nEDM Overview and requirements. Presented at *Meeting at PTB Berlin*, Berlin, Germany, 2019-09-17 - 2019-09-17. (LA-UR-19-29478)

Ito, T. Neutron Electric Dipole Moment Search Experiments in the US. Presented at *Atomic nuclei as laboratories for BSM physics*, Trento, Italy, 2019-04-15 - 2019-04-18. (LA-UR-19-23340)

Ito, T. nEDM at LANL. Presented at *Snowmass: Workshop on Electric and Magnetic Dipole Moments*, Los Alamos, New Mexico, United States, 2020-09-15 - 2020-09-15. (LA-UR-20-27227)

Ito, T. UCN Future at LANSCE. Presented at *LANSCE Future Spring Workshop*, Los Alamos, New Mexico, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-24476)

Ito, T. UCN Source in Area A. Presented at *LANSCE Futures Spring Workshop 2021: Area A*, Los Alamos, New Mexico, United States, 2021-06-01 - 2021-06-01. (LA-UR-21-25187)

Ito, T. Fundamental neutron physics at Los Alamos National Laboratory. Presented at *Seminar at Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Italy.*, Frascati, Italy, 2022-03-16 - 2022-03-16. (LA-UR-22-22471)

Ito, T., T. Bhattacharya and S. Clayton. LDRD 20190041DR: 3rd year project appraisal. . (LA-UR-21-20898)

Park, S. Flavor diagonal matrix elements. Presented at *USQCD All Hands' Meeting 2021*, Cambridge, Massachusetts, United States, 2021-04-30 - 2021-05-01. (LA-UR-21-24213)

Park, S., R. Gupta, T. Bhattacharya, B. Yoon, S. Mondal, H. W. Lin and R. Zhang. Flavor diagonal nucleon chargese. Presented at *The 38th international symposium on lattice field theory*, Cambridge, Massachusetts, United States, 2021-07-26 - 2021-07-30. (LA-UR-21-27171)

Park, S., T. Bhattacharya, R. Gupta, B. Yoon, Y. Jang, K. Orginos, D. Richards, H. Lin and B. Joo. Nucleon Charges and Form Factors on clover lattices. Presented at *the 37th international conference on lattice field theory*, Wuhan, China, 2019-06-16 - 2019-06-22. (LA-UR-19-25549)

Yoon, B. Lattice QCD for EDMs: Current Status and Future Prospects. Presented at *Workshop on Electric and Magnetic Dipole Moments*, Virtual, New Mexico, United States, 2020-09-15 - 2020-09-15. (LA-UR-20-27473)

Yoon, B. Prediction of lattice QCD observables using machine learning. Presented at *Machine learning techniques in lattice QCD*, Online, Germany, 2021-05-24 - 2021-05-28. (LA-UR-21-24915)

Yoon, B. Machine Learning Prediction and Compression of Lattice QCD Observables. Presented at *Machine Learning for High Energy Physics, on and off the Lattice*, Trento, Italy, 2021-09-27 - 2021-09-27. (LA-UR-21-29432)

Yoon, B., N. T. T. Nguyen-Fotiadis, G. Kenyon, C. C. Chang and E. Rrapaj. Prediction and compression of lattice QCD data using ML algorithms on quantum annealer. Presented at *The 38th International Symposium on Lattice Field Theory*, Cambridge, Massachusetts, United States, 2021-07-26 - 2021-07-30. (LA-UR-21-27155)

Yoon, B., T. Bhattacharya, R. Gupta and V. Cirigliano. Neutron Electric Dipole Moment from QCD and BSM using Clover-on-HISQ. Presented at *Lattice 2019*, Wuhan, China, 2019-06-16 - 2019-06-22. (LA-UR-19-25441)

Yoon, B., T. Bhattacharya, V. Cirigliano, R. Gupta, M. Hoferichter, Y. Jang, B. Joo, H. W. Lin, E. Mereghetti, S. Mondal, S. Park and F. Winter. Nucleon Charges from Lattice QCD. Presented at *A Virtual Tribute to Quark Confinement and the Hadron Spectrum 2021*, Stavanger, Norway, 2021-08-02 - 2021-08-02. (LA-UR-21-27481)

Yoon, B., T. Bhattacharya and R. Gupta. Machine learning regression and error quantification for lattice QCD Monte Carlo observables. Presented at *A Virtual Tribute to Quark Confinement and the Hadron Spectrum 2021*, Stavanger, Norway, 2021-08-02 - 2021-08-06. (LA-UR-21-27372)

Posters

Yoon, B., N. T. T. Nguyen, T. Bhattacharya, G. Kenyon and R. Gupta. Quantum Machine Learning for Lattice QCD. Presented at *2019 Quantum Information Science (QIS) Kick Off Principal Investigators' Meeting*, Rockville, Maryland, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20388)

Yoon, B., N. T. T. Nguyen-Fotiadis, T. Bhattacharya, R. Gupta and G. Kenyon. Quantum Machine Learning for Lattice QCD. Presented at *Quantum Information Science (QIS) Principal Investigator (PI) Meeting*, Washington, District Of Columbia, United States, 2020-03-12 - 2020-03-13. (LA-UR-20-22302)

Convincing Search for Sterile Neutrinos at Lujan

Richard Van De Water
20190098DR

Project Description

This project will have a significant impact on the Laboratory, as it brings experimental neutrino physics back to the place it started in the 1950's with the Nobel Prize winning discovery of the neutrino by Cowen and Reines. High profile Research & Development attracts the brightest and best students, with most of our postdocs going on to successful careers at Los Alamos and at other national labs and universities. We are developing a significant external collaboration of world leading researchers in neutrino physics, who will bring talented students and postdocs to work on the experiment. Fermi National Accelerator Laboratory (FNAL) has expressed support for the project and is allowing a staff scientist to participate. The long-term goal is to develop a robust and flexible neutrino facility to attract new National Science Foundation/Department of Energy basic science funding to support novel neutrino experiments and to test technologies for future short- and long- baseline programs. These element are all important to Los Alamos for producing a stronger scientific base, and hence by extension, to DOE/National Nuclear Security Administration, and the nation.

Publications

Journal Articles

Spier Moreira Alves, D., W. C. I. Louis and P. deNiverville. Quasi-Sterile Neutrinos from Dark Sectors I. BSM matter effects in neutrino oscillations and the short-baseline anomalies. Submitted to *Journal of High Energy Physics*. (LA-UR-22-20015)

Spier Moreira Alves, D., W. C. I. Louis and P. deNiverville. Quasi-Sterile Neutrinos from Dark Sectors I. BSM matter effects in neutrino oscillations and the short-baseline anomalies. Submitted to *Journal of High Energy Physics*. (LA-UR-22-20015)

*Gupta, R., B. joo, T. Bhattacharya, S. Park, B. Yoon, S. Mondal and F. Winter. Nucleon momentum fraction, helicity and transversity from 2+1-flavor lattice QCD. 2021. *Journal of High Energy Physics*. **2021** (4): 44. (LA-UR-20-28586 DOI: 10.1007/JHEP04(2021)044)

Gupta, R., b. Joo, T. Bhattacharya, B. Yoon, S. Park, S. Mondal, F. winter and Y. C. Jang. Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD. Submitted to *Physical Review D*. (LA-UR-21-20526)

I. Louis, W. C. and R. G. Van De Water. The Darkest Pariclcs. Submitted to *Scientific American*. (LA-UR-21-22417)

Thornton, R. T., A. A. Aguilar-Arevalo, J. G. Boissevain, S. Biedron, J. Conrad, P. deNiverville, J. C. D'Olivo, J. R. Distel, E. Dunton, B. Dutta, D. Fields, M. Gold, E. Guardincerri, E. Huang, W. C. I. Louis, R. Mahapatra, S. Maludze, J. Mirabal-Martinez, H. Neog, V. Pandey, D. C. Poulson, H. Ray, E. L. Renner, T. J. Schaub, M. H. Shaevitz, D. Smith, W. E. Sondheim, D. Spier Moreira Alves, C. E. Taylor, M. Tripathi, W. H. W. Thompson, R. Van Berg, R. G. Van De Water and S. Verma. Dark Matter Search using the CCM-120 Detector. Submitted to *Physical Review D*. (LA-UR-21-24983)

Thornton, R. T., A. A. Aguilar-Arevalo, J. G. Boissevain, S. Biedron, J. Conrad, P. deNiverville, J. C. D'Olivo, J. R. Distel, E. Dunton, B. Dutta, D. Fields, M. Gold, E. Guardincerri, E. Huang, W. C. I. Louis, R. Mahapatra, S. Maludze, J. Mirabal-Martinez, H. Neog, V. Pandey, D. C. Poulson, H. Ray, E. L. Renner, T. J. Schaub, M. H. Shaevitz, D. Smith, W. E. Sondheim, D. Spier Moreira Alves, C. E. Taylor, M. Tripathi, W. H. W. Thompson, R. Van Berg, R. G. Van De Water and S. Verma. Dark Matter Search using the CCM-120 Detector. Submitted to *Physical Review D*. (LA-UR-21-24983)

Thornton, R. T., A. A. Aguilar-Arevalo, J. G. Boissevain, S. Biedron, J. Conrad, P. deNiverville, J. C. D'Olivo, J. R. Distel, E. Dunton, B. Dutta, D. Fields, M. Gold, E. Guardincerri, E. Huang, W. C. I. Louis, R. Mahapatra, S. Maludze, J. Mirabal-Martinez, H. Neog, V. Pandey, D. C. Poulson, H. Ray, E. L. Renner, T. J. Schaub, M. H. Shaevitz, D. Smith, W. E. Sondheim, D. Spier Moreira Alves, C. E. Taylor, M. Tripathi, W. H. W. Thompson, R. Van Berg, R. G. Van De Water and S. Verma. Dark Matter Search using the CCM-120 Detector. Submitted to *Physical Review D*. (LA-UR-21-24983)

Thornton, R. T., R. G. Van De Water and W. C. I. Louis. First Leptophobic Dark Matter Search with Coherent CAPTAIN-Mills. Submitted to *Physical Review Letters*. (LA-UR-21-28552)

Thornton, R. T., R. G. Van De Water and W. C. I. Louis. First Leptophobic Dark Matter Search with Coherent CAPTAIN-Mills. Submitted to *Physical Review Letters*. (LA-UR-21-28552)

Thornton, R. T., R. G. Van De Water and W. C. I. Louis. First Leptophobic Dark Matter Search with Coherent CAPTAIN-Mills. Submitted to *Physical Review Letters*. (LA-UR-21-28552)

Van De Water, R. G., W. C. I. Louis, D. Spier Moreira Alves, P. deNiverville and R. T. Thornton. Axion Like Particles at Coherent CAPTAIN-Mills. Submitted to *Physical Review Letters*. (LA-UR-21-28474)

Van De Water, R. G. and W. C. I. Louis. Sterile Neutrinos. Submitted to *Scientific American*. (LA-UR-19-32514)

deNiverville, P., L. Buonocore and C. Frugiuele. The hunt for sub-GeV dark matter at neutrino facilities: a survey of past and present experiments. Submitted to *Journal of High Energy Physics*. (LA-UR-19-32644)

Conference Papers

Gupta, R., M. Hoferichter, T. Bhattacharya, V. Cirigliano, E. Mereghetti, Y. C. Jang, B. Joo, F. Winter, B. Yoon, S. Park and S. Mondal. Excited states and precision results for nucleon charges and form factor. Presented at *The 38th International Symposium on Lattice Field Theory, LATTICE2021 26th-30th July, 2021 Zoom/Gather@Massachusetts Institute of Technology*. (Cambridge, Massachusetts, United States, 2021-07-26 - 2021-07-30). (LA-UR-21-32449)

Reports

I. Louis, W. C., R. G. Van De Water, R. T. Thornton, E. Huang, S. Gollapinni and J. Mirabal-Martinez. Updated MiniBooNE Neutrino Oscillation Results with Increased Data and New Background Studies. Unpublished report. (LA-UR-20-24753)

Toups, M., S. J. Brice, J. Eldred, R. Harnik, K. Kelly, T. Kobilarcik, G. Krnjaic, P. Machado, Z. Pavlovic, B. Pellico, J. Zettlemoyer, B. Zwaska, R. G. Van De Water, P. deNiverville, W. C. I. Louis, R. T. Thornton, B. Batell, B. R. Littlejohn, P. Snopok, M. H. Shaevitz, R. Tayloe, T. Hapitas, D. Tuckler and Y. Zhang. PIP2-BD: GeV Proton Beam Dump at Fermilab's PIP-II Linac. Unpublished report. (LA-UR-22-22447)

Van De Water, R. G., M. Toups, B. Batell, S. J. Brice, P. deNiverville, J. Eldred, A. Fava, K. J. Kelly, T. Kobilarcik, W. C. I. Louis, P. Machado, B. Pellico, J. Spitz, R. Tayloe, R. T. Thornton, Z. Pavlovic and J. Zettlemoyer. SBN-BD: O(10 GeV) Proton Beam Dump at Fermilab's PIP-II Linac. Unpublished report. (LA-UR-22-22524)

deNiverville, P., R. G. Van De Water, O. S. Tomalak, J. Arrington, J. Barrow, B. Batell, R. Bernstein, N. Blinov, S. J. Brice, R. Culbertson, J. Eldred, A. Fava, L. Fields, A. Friedland, A. Gaponenko, C. Gatto, S. Gori, R. Harnik, R. J. Hill, D. M. Kaplan, K. J. Kelly, M. Kiburg, T. Kobilarcik, G. Krnjaic, G. Lee, B. R. Littlejohn, W. C. I. Louis, P. Machado, A. Mazzacane, P. Merkel, W. M. Morse, D. Neuffer, E. Niner, Z. Pavlovic, W. Pellico, R. Plestid, M. Pospelov, E. Prebys, Y. Semertzidis, M. H. Shaevitz, P. Snopok, M. J. Syphers, R. Tayloe, R. T. Thornton, M. Toups, N. Tran, K. Yonehara, J. Zettlemoyer, Y. Zhong and R. Zwaska. Physics Opportunities for the Fermilab Booster Replacement. Unpublished report. (LA-UR-22-21987)

Presentation Slides

Spier Moreira Alves, D. New Physics Signals In Hadronic Processes. . (LA-UR-21-22706)

Spier Moreira Alves, D. HEP Site Review Presentation. Presented at *DOE HEP Site Review*, Los Alamos, New Mexico, United States, 2021-07-06 - 2021-07-08. (LA-UR-21-25967)

Edwards, T. R. Searching for Sterile Neutrinos and Accelerator Produced Dark Matter with Coherent CAPTAIN Mills. Presented at *APS April Meeting*, Washington, District Of Columbia, United States, 2020-04-18 - 2020-04-18. (LA-UR-20-22990)

Guardincerri, E. Viewgraphs for HPC w20_ccm_lanl annual report. . (LA-UR-21-21898)

Gupta, R. Lattice QCD at LANL (2020 PR). . (LA-UR-21-22424)

Gupta, R. Excited states and precision results for nucleon charges and form factors. Presented at *38 International Symposium on Lattice Field Theory, 2021*, Boston (virtual), Massachusetts, United States, 2021-07-26 - 2021-07-26. (LA-UR-21-27234)

Gupta, R., H. Lin, B. Yoon, S. Mondal, T. Bhattacharya and S. Park. Flavor diagonal matrix elements. Presented at *USQCD all hands meeting*, Boston (virtual), Massachusetts, United States, 2021-04-30 - 2021-04-30. (LA-UR-21-24214)

Gupta, R., M. Hoferichter, E. Mereghetti, T. Bhattacharya, B. Yoon and S. Park. The pion–nucleon sigma term from lattice QCD. Presented at *Chiral Dynamics 2021*, Beijing, China, 2021-11-15 - 2021-11-15. (LA-UR-21-31181)

Gupta, R., T. Bhattacharya, B. Yoon, S. Park, H. W. Lin, B. Joo and F. Winter. Nucleon isovector momentum fraction, helicity and transversity moment using Lattice QCD. Presented at *The 38th International Symposium on Lattice Field Theory*, Boston, Massachusetts, United States, 2021-07-26 - 2021-07-26. (LA-UR-21-27204)

Renner, E. L. Design of the Coherent CAPTAIN Mills (CCM) Roof Shielding Package. . (LA-UR-21-21086)

Schaub, T. J. Searching for Sterile Neutrinos and Accelerator Produced Dark Matter with the Coherent CAPTAIN-Mills (CCM) Detector at the Los Alamos Neutron Science Center. Presented at *APS April Meeting 2021*, Los Alamos, New Mexico, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-20576)

W. Thompson, W. H. Coherent Captain Mills CCM 200 Upgrade. Presented at *SULI Presentation and Peer Review*, Los Alamos, New Mexico, United States, 2021-05-05 - 2021-05-05. (LA-UR-21-27778)

W. Thompson, W. H. Dark Matter Search at Coherent CAPTAIN Mills. Presented at *Magnificent CEvNS*, Los Alamos, New Mexico, United States, 2021-10-06 - 2021-10-06. (LA-UR-21-29913)

W. Thompson, W. H. Coherent Captain Mills UNM Presentation. Presented at *UNM Talk*, Albuquerque, New Mexico, United States, 2022-03-02 - 2022-03-02. (LA-UR-22-21825)

Thornton, R. T. and E. L. Renner. Lessons Learned From CCM120/Upgrades to the Coherent CAPTAIN Mills experiment for the upcoming CCM200 run. Presented at *Magnificent CEvNS Workshop*, Cyberspace, North Carolina, United States, 2020-11-16 - 2020-11-20. (LA-UR-20-29390)

Van De Water, R. G. Searching for Sterile Neutrinos with the Coherent CAPTAIN-Mills Detector at the Los Alamos Neutron Science Center. Presented at *APS April Meeting 2019*, Denver, Colorado, United States, 2019-04-13 - 2019-04-13. (LA-UR-19-24037)

Van De Water, R. G. The Coherent CAPTAIN-Mills Experiment. Presented at *HEP Site Review*, Los Alamos, New Mexico, United States, 2021-07-07 - 2021-07-07. (LA-UR-21-25957)

Van De Water, R. G. LANSCE Intense Pulsed Proton Source Search for the Dark Sector : The Coherent CAPTAIN-Mills Experiment. Presented at *Duke University Seminar*, Durham, North Carolina, United States, 2021-11-02 - 2021-11-02. (LA-UR-21-30818)

A New Era of Nuclear Physics at the Electron-Ion Collider

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20200022DR

Project Description

A United States-based high-intensity Electron Ion Collider (EIC) can uniquely address profound questions about nucleons - neutrons and protons - and how they are assembled to from the nuclei of atoms. The EIC will provide the ultimate microscope to determine both the static properties of nucleons and nuclei, as well as how matter and energy can be transported through a strongly interacting quantum mechanical environment. The production and propagation of long-lived heavy subatomic particles is a unique and critical part of this planned decade-long research program. The EIC is an essential component of the Department of Energy's mission to understand all forms of nuclear matter, and this project will enable the use of jets of heavy particles to accomplish this task. It will ensure that the United States maintains its leadership in state-of-the art detector technology, high performance and quantum computing. A secondary long-term benefit from the project is high-resolution, ultra-fast, radiation hard silicon technology that can find applications in dynamic experiments that help certify our nuclear stockpile. Current and future experimental imaging efforts using existing light sources such as the Linac Coherent Light Source and the Advanced Photon Source can also benefit from faster imaging detectors.

Publications

Journal Articles

*Brueser, R., Z. L. Liu and M. Stahlhofen. Three-loop soft function for heavy-to-light quark decays. 2021. *Journal of High Energy Physics*. **2020** (3): 71. (LA-UR-20-28943 DOI: 10.1007/JHEP03(2020)071)

Caro, M., H. Huang, M. V. S. Cerezo de la Roca, K. Sharma, A. T. Sornborger, L. Cincio and P. J. Coles. Generalization in quantum machine learning from few training data. Submitted to *Nature Physics*. (LA-UR-21-31086)

Caro, M., L. Cincio, J. Gibbs, Z. P. Holmes, N. A. Ezzell, H. Huang, A. T. Sornborger and P. J. Coles. Dynamical simulation via quantum machine learning with provable generalization. Submitted to *PRL*. (LA-UR-22-20965)

Gibbs, J., K. Gili, Z. P. Holmes, B. Commeau, A. T. Arrasmith, L. Cincio, A. T. Sornborger and P. J. Coles. Long-time simulations with high fidelity on quantum hardware. Submitted to *arXiv, PRX Quantum*. (LA-UR-21-21053)

V. I. Li, H. *., H. Li and I. Vitev. Jet charge modification in dense QCD matter. Submitted to *PoS - Proceedings of Science*. (LA-UR-20-28020 DOI: 10.22323/1.387.0145)

. V. I. Li, H. T., H. T. Li and I. Vitev. Nuclear Matter Effects on Jet Production at Electron-Ion Colliders. 2021. *Physical Review Letters*. **126 (25): 252001. (LA-UR-20-28006 DOI: 10.1103/PhysRevLett.126.252001)

Li, H., I. M. Vitev and Y. J. Zhu. Transverse-Energy-Energy Correlations in Deep Inelastic Scattering. Submitted to *Journal of High Energy Physics*. (LA-UR-20-24408)

Li, H., Z. Liu and I. M. Vitev. Heavy meson tomography of cold nuclear matter at the electron-ion collider. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-20-28936)

*Li, H. and I. M. Vitev. Jet charge modification in finite QCD matter. 2020. *Physical Review D*. **101** (7): 076020. (LA-UR-19-30442 DOI: 10.1103/PhysRevD.101.076020)

*Li, X., I. Vitev, M. Brooks, L. Cincio, J. M. Durham, M. Graesser, M. X. Liu, A. Morreale, D. Neill, C. da Silva, W. E. Sondheim and B. Yoon. A New Heavy Flavor Program for the Future Electron-Ion Collider. *EPJ Web of Conferences*. **235**: 04002. (LA-UR-20-21411 DOI: 10.1051/epjconf/202023504002)

Li, X., J. M. Durham, M. L. Brooks, E. L. Renner, W. E. Sondheim, C. J. Prokop, A. Morreale and Y. Corrales Morales. Forward silicon vertex/tracking detector design and R&D for the future Electron-Ion Collider. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-30898 DOI: 10.22323/1.380.0084)

*Liu, Z. L., B. Mecaj, M. Neubert, X. Wang and S. Fleming. Renormalization and scale evolution of the soft-quark soft function. 2021. *Journal of High Energy Physics*. **2020** (7): 104. (LA-UR-20-28935 DOI: 10.1007/JHEP07(2020)104)

*Liu, Z. L. and M. Neubert. Two-loop radiative jet function for exclusive B-meson and Higgs decays. 2020. *Journal of High Energy Physics*. **2020** (6): 60. (LA-UR-20-28934 DOI: 10.1007/JHEP06(2020)060)

Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in Soft-

Collinear Effective Theory. Submitted to *Physical Review Letters*. (LA-UR-20-28937)

Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in h \xe2\x86\x92\xce\xb3\xce\xb3 Decay: II. Renormalization and Scale Evolution. Submitted to *Journal of High Energy Physics*. (LA-UR-20-28938)

Liu, Z. and M. Neubert. Factorization at Subleading Power and Endpoint-Divergent Convolutions in h \xe2\x86\x92 \xce\xb3\xce\xb3 Decay. Submitted to *Journal of High Energy Physics*. (LA-UR-20-28704)

Liu, Z. and M. Stahlhofen. Three-loop soft function for energetic electroweak boson production at hadron colliders. Submitted to *Journal of High Energy Physics*. (LA-UR-20-28939)

Neill, D. A., N. Sato and F. Ringer. Leading jets and the jet energy loss – a parton shower approach at NLL. Submitted to *Journal of High Energy Physics*. (LA-UR-21-22574)

Neill, D. A., Y. Makris, F. Ringer, N. Sato and M. Arratia. Asymmetric jet clustering in deep-inelastic scattering. Submitted to *Physical Review Letters*. (LA-UR-20-24434)

S. Cerezo de la Roca, M. V., A. T. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio and P. J. Coles. Variational Quantum Algorithms. Submitted to *Nature Reviews Physics*. (LA-UR-20-30142)

Saxena, A. B., A. S. Rodrigues, R. M. Ross, V. V. Konotop and P. G. Kevrekidis. Nonlinear Anti-(Parity-Time) symmetric dimer. Submitted to *Frontiers in Physics*. (LA-UR-22-20440)

Saxena, A. B., R. Balakrishnan and R. Dandoloff. Exact Hop \xe2\x80\x80ons in a 3D Heisenberg Ferromagnet. Submitted to *Physical Review Letters*. (LA-UR-22-20711)

Saxena, A. B. and A. Khare. Kink Solutions With Power Law Tails. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-21-31062)

Saxena, A. B. and A. Khare. Novel Superposed Kink and Pulse Solutions for $\\phi^4$, MKdV, NLS and Other Nonlinear Equations. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-22-20992)

Saxena, A. B. and A. Khare. Superposed Hyperbolic Kink and Pulse Solutions of Coupled $\\phi^4$, NLS and MKdV Equations. Submitted to *Physics Letters. Section A: General, Atomic and Solid State Physics*. (LA-UR-22-21628)

Sharma, K., M. V. S. Cerezo de la Roca, L. Cincio and P. J. Coles. Trainability of Dissipative Perceptron-Based Quantum Neural Networks. Submitted to *Physical Review Letters*. (LA-UR-20-23484)

Sornborger, A. T., B. A. Commeau, M. V. S. Cerezo de la Roca, Z. P. Holmes, L. Cincio and P. J. Coles. \xef\xbb\xbfVariational Hamiltonian Diagonalization for Dynamical Quantum Simulation. Submitted to *Quantum*. (LA-UR-20-26827)

Vitev, I. M., H. Li and Y. J. Zhu. Transverse-Energy-Energy Correlations in Deep Inelastic Scattering. Submitted to *Journal of High Energy Physics*. (LA-UR-20-28010)

Vitev, I. M., H. Li and Y. Makris. Energy-energy correlators in Deep Inelastic Scattering. Submitted to *Physical Review D*. (LA-UR-21-21419)

Vitev, I. M., H. Li and Z. Liu. Heavy meson tomography of cold nuclear matter at the electron-ion collider. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-20-28004)

Vitev, I. M., Z. Liu and H. Li. Heavy flavor jet production and substructure in electron-nucleus collisions. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-21-28557)

Wong, C. and X. Li. A Forward Silicon Tracker for the Future Electron-ion Collider Experiments. Submitted to *Proceedings*. (LA-UR-22-21912)

*Yoon, B. A machine learning approach for efficient multi-dimensional integration. 2021. *Scientific Reports*. **11** (1): 18965. (LA-UR-20-27161 DOI: 10.1038/s41598-021-98392-z)

Zhang, R., H. Lin and B. Yoon. Probing nucleon strange and charm distributions with lattice QCD. Submitted to *arXiv*. (LA-UR-20-23850)

*Zhang, R., Z. Fan, R. Li, H. Lin and B. Yoon. Machine-learning prediction for quasiparton distribution function matrix elements. 2020. *Physical Review D*. **101** (3): 034516. (LA-UR-19-30235 DOI: 10.1103/PhysRevD.101.034516)

Conference Papers

Li, H. Jet charge in heavy-ion collisions. Presented at *https://indico.cern.ch/event/761800/*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-09). (LA-UR-20-21864)

Li, X. Heavy flavor and jet studies for the future Electron-Ion Collider. Presented at *10th International Conference on Hard and Electromagnetic Probes of High-Energy Nuclear Collisions (online)*. (Austin, Texas, United States, 2020-05-31 - 2020-06-05). (LA-UR-20-25450)

Li, X. Open heavy flavor and jet studies for the future Electron-Ion Collider. Presented at *EIC opportunities for Snowmass 2021, heavy flavor session*. (Upton, New York, United States, 2021-01-25 - 2021-01-29). (LA-UR-21-21900)

Li, X. Heavy Flavor and Jet Studies for the Future Electron-Ion Collider. Presented at *XXVIII International Workshop on Deep-Inelastic Scattering and Related Subjects*. (Stonybrook, New York, United States, 2021-04-12 - 2021-04-16). (LA-UR-21-26415)

Li, X., A. Morreale and W. E. Sondheim. Silicon pixel-based Particle Vertex and Tracking Detectors towards the USElectron Ion Collider. Presented at *Silicon pixel-based Particle Vertex and Tracking Detectors towards the*

USElectron Ion Collider workshop. (Newport News, Virginia, United States, 2020-09-02 - 2020-09-04). (LA-UR-21-21344)

Li, X., C. Wong, I. M. Vitev and J. M. Durham. Electron Ion Collider for High Energy Physics. Presented at *EIC opportunities for Snowmass*. (Stonybrook, New York, United States, 2021-01-25 - 2021-01-29). (LA-UR-22-22110)

Books/Chapters

Lee, C., I. M. Vitev, R. Boussarie, J. W. Qiu, I. W. Stewart, T. Mehen, M. Burkardt, M. Constantinou, W. Detmold, M. Ebert, M. Engelhardt, S. Fleming, L. Gamberg, X. Ji, Z. B. Kang, K. F. Liu, S. Liuti, A. Metz, J. Negele, D. Pitonyak, A. Prokudin, A. Rajan, M. Schlegel, P. Shanahan, P. Schweitzer, A. Tarasov, R. Venugopalan, F. Yuan and Y. Zhao. TMD Handbook: A modern introduction to the physics of Transverse Momentum Dependent distributions. (LA-UR-21-20798)

Da Silva, C. L., J. M. Durham, C. Lee, X. Li, M. X. Liu, A. Morreale, W. E. Sondheim, I. M. Vitev, B. Surrow, R. Milner, A. Dumitru, O. Evdomikov, A. Metz, C. Mu\xc3\xb1oz Camacho, K. Barish, T. Horn, P. Jones, S. Dalla Torre, M. Diefenthaler and C. Wong. EIC Yellow Report. (LA-UR-21-20953)

Reports

Cincio, L. Error mitigation with Clifford quantum-circuit data. Unpublished report. (LA-UR-22-21698)

Li, X. Expression of Interest in Contributions to the Electron-Ion Collider: Forward Silicon Vertex/Tracker Developments. Unpublished report. (LA-UR-20-28718)

Li, X., C. Wong, M. L. Brooks, J. M. Durham, M. X. Liu, A. Morreale, C. L. Da Silva and W. E. Sondheim. A Proposed Forward Silicon Tracker for the Future Electron-Ion Collider and Associated Physics Studies. Unpublished report. (LA-UR-20-26642)

Vitev, I. M., D. A. Neill, G. Vita and H. X. Zhu. Energy-Energy Correlators for Precision QCD. Unpublished report. (LA-UR-22-22441)

Vitev, I. M., J. Qiu, L. Cincio, D. A. Neill and B. Yoon. Toward Quantum Computation of Hadronization in QCD. Unpublished report. (LA-UR-21-24757)

Presentation Slides

Caro, M., H. Huang, M. V. S. Cerezo de la Roca, K. Sharma, A. T. Sornborger, L. Cincio and P. J. Coles. Generalization in quantum machine learning from few training data. Presented at *Quantum Techniques in Machine Learning 2021*, Tokyo, Japan, 2021-11-08 - 2021-11-08. (LA-UR-21-31075)

Cincio, L. QCD on quantum computers. Presented at *LDRD feasibility review*, Los Alamos, New Mexico, United States, 2020-02-06 - 2020-02-06. (LA-UR-20-21128)

Cincio, L. Fast forwarding QFTs on qauntum computers. Presented at *LDRD DR appraisal*, on-line, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-30035)

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Durham, J. M. Heavy flavor physics at the EIC. Presented at *LPC Workshop on Physics Connections between the LHC and EIC*, Batavia, Illinois, United States, 2019-11-13 - 2019-11-13. (LA-UR-19-31583)

Durham, J. M. A New Era of Nuclear Physics at the Electron Ion Collider: Experimental Detail. . (LA-UR-20-21174)

Durham, J. M. Probing the Structure of Exotic Hadrons at the EIC. Presented at *Snowmass 2020*, Batavia, Illinois, United States, 2020-08-04 - 2020-08-04. (LA-UR-20-25885)

Durham, J. M. Probing the Structure of Exotic Hadrons at the EIC. Presented at *EIC Opportunities for Snowmass*, Stony Brook, New York, United States, 2021-01-25 - 2021-01-25. (LA-UR-21-20652)

Li, X. The proposed forward silicon tracking design and readout needs for the EIC. Presented at *Streaming Readout V, Developing a common, community-wide standard for streaming readout*, Upton, New York, United States, 2019-11-13 - 2019-11-15. (LA-UR-19-31272)

Li, X. Jets and heavy flavor at EIC as an important part of its physics program - new developments/progress at LANL. Presented at *EIC Yellow Report Kick-Off meeting*, Cambridge, Massachusetts, United States, 2019-12-12 - 2019-12-13. (LA-UR-19-32203)

Li, X. New heavy flavor program for the future Electron Ion Collider. Presented at *UIC physics division seminar*, Chicago, Illinois, United States, 2019-10-01 - 2019-10-01. (LA-UR-19-29804)

Li, X. New Heavy Flavor Program for the Future Electron Ion Collider. Presented at *Fall Meeting of the Division of Nuclear Physics of the American Physical Society*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30295)

Li, X. EIC silicon tracking detector R&D opportunities. Presented at *Phone meeting about the HV-MAPS for the silicon tracking detector at the future EIC*, Los Alamos, New Mexico, United States, 2020-01-13 - 2020-01-13. (LA-UR-20-20219)

Li, X. EIC physics program status and plans at Los Alamos National Laboratory. Presented at *UC EIC Consortium meeting*, Riverside, California, United States, 2020-01-16 - 2020-01-17. (LA-UR-20-20480)

Li, X. LDRD DR 20200022DR Feasibility Review - EIC DR experimental overview. Presented at *The LDRD DR 20200022DR Feasibility Review*, Los Alamos, New Mexico, United States, 2020-02-06 - 2020-02-06. (LA-UR-20-21095)

Li, X. The EIC tracking detector thoughts. Presented at *EIC yellow report tracking group*, Upton, New York, United States, 2020-02-13 - 2020-02-13. (LA-UR-20-21468)

Li, X. New Heavy Flavor and Jet program for the EIC. Presented at *Invited seminar at Jefferson Laboratory*, Newport News, Virginia, United States, 2020-02-19 - 2020-02-21. (LA-UR-20-21677)

Li, X. LANL contribution plan to the EIC Jets and Heavy Flavor working group. Presented at *The EIC Yellow Report Jets and Heavy Flavor working group meeting*, Upton, New York, United States, 2020-02-26 - 2020-02-26. (LA-UR-20-21862)

Li, X. Forward silicon tracking studies for the EIC Yellow Report preparation. Presented at *The 1st EIC Yellow Report Workshop at Temple University*, Philadelphia, Pennsylvania, United States, 2020-03-19 - 2020-03-21. (LA-UR-20-22451)

Li, X. Heavy Flavor and jet studies for the future Electron Ion Collider. Presented at *APS April meeting 2020*, Washington, District Of Columbia, United States, 2020-04-18 - 2020-04-21. (LA-UR-20-22978)

Li, X. Open heavy flavor study updates for the EIC yellow report preparation. Presented at *EIC yellow report jets and heavy flavor WG meeting*, Upton, New York, United States, 2020-05-04 - 2020-05-04. (LA-UR-20-23348)

Li, X. For the EIC silicon tracking detector discussions. Presented at *Joint LANL and LBNL EIC simulation and hardware meeting*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-18. (LA-UR-20-23688)

Li, X. Heavy flavor and jet studies for the future Electron-Ion Collider. Presented at *The 10th edition of the Hard and Electromagnetic Probes International Conference series*, Austin, Texas, United States, 2020-06-01 - 2020-06-05. (LA-UR-20-23938)

Li, X. Requirements from EIC forward heavy flavor studies. Presented at *SILICON PIXEL-BASED PARTICLE VERTEX AND TRACKING DETECTORS TOWARDS THE US ELECTRON ION COLLIDER WORKSHOP*, Newport News, Virginia, United States, 2020-09-02 - 2020-09-04. (LA-UR-20-26812)

Li, X. Heavy Flavor and jet studies for the future Electron Ion Collider. Presented at *2020 Fall Meeting of the APS Division of Nuclear Physics*, New Orleans, Louisiana, United States, 2020-10-29 - 2020-11-01. (LA-UR-20-28717)

Li, X. Heavy Flavor and jet studies for the future Electron-Ion Collider. Presented at *Jets for 3D imaging online workshop*, Riverside, California, United States, 2020-11-23 - 2020-11-25. (LA-UR-20-29562)

Li, X. Heavy Flavor and jet studies for the future Electron-Ion Collider. Presented at *The VI-th International Conference on the Initial Stages of High-Energy Nuclear Collisions*, Rehovot, Israel, 2021-01-10 - 2021-01-15. (LA-UR-21-20030)

Li, X. LGAD (AC-LGAD) detector R&D status and plan at LANL. Presented at *LGAD Consortium Detector Projects and Interests*, Houston, Texas, United States, 2021-02-03 - 2021-02-03. (LA-UR-21-20942)

Li, X. Subsystem Interest - Forward Silicon Vertex/Tracking Detector for EIC. Presented at *Kick-off Meeting for an EIC Detector at IP6 (EIC@IP6)*, Upton, New York, United States, 2021-03-12 - 2021-03-13. (LA-UR-21-22387)

Li, X. Exploring hadronization through heavy flavor probes at the Electron-Ion Collider. Presented at *LBNL HIT seminar*, Berkeley, California, United States, 2021-03-16 - 2021-03-16. (LA-UR-21-22484)

Li, X. Heavy flavor and jet studies for the future Electron-Ion Collider. Presented at *XXVIII International Workshop on Deep-Inelastic Scattering and Related Subjects (DIS2021)*, Stony Brook, New York, United States, 2021-04-12 - 2021-04-16. (LA-UR-21-23270)

Li, X. Open heavy flavor and jet studies for the future Electron-Ion Collider. Presented at *APS April meeting 2021*, Washington, District Of Columbia, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23413)

Li, X. ECCE Tracking detector progress report. Presented at *EICUG Summer 2021 Meeting*, Riverside, California, United States, 2021-08-02 - 2021-08-06. (LA-UR-21-27260)

Li, X. New Hard Probe Studies for the future Electron-Ion Collider. Presented at *INT21 workshop "Probing QCD at High Energy and Density with Jets"*, Seattle, Washington, United States, 2021-07-26 - 2021-08-27. (LA-UR-21-28316)

Li, X. Forward silicon vertex/tracking detector design and R&D for the future Electron-Ion Collider. Presented at *22nd edition Particles and Nuclei International Conference (PANIC2021)*, Lisbon, Portugal, 2021-09-05 - 2021-09-10. (LA-UR-21-28808)

Li, X. Explore hadronization through heavy flavor probes at the future Electron-Ion Collider. Presented at *APS DNP 2021 meeting*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-14. (LA-UR-21-29824)

Li, X. Exploring hadronization through heavy flavor probes at the Electron-Ion Collider. Presented at *Georgia State University Physics Seminar*, Atlanta, Georgia, United States, 2021-11-02 - 2021-11-02. (LA-UR-21-30612)

Li, X. LGAD (AC-LGAD) detector R&D at LANL for the future Electron-Ion Collider. Presented at *EIC LGAD Consortium meeting*, Upton, New York, United States, 2021-11-01 - 2021-11-01. (LA-UR-21-30528)

Li, X. Open heavy flavor study updates for the EIC yellow report preparation. Presented at *EIC yellow report jets and heavy flavor working group weekly meeting*, Upton, New York, United States, 2020-04-06 - 2020-04-06. (LA-UR-20-22742)

Li, X. LANL EIC studies and plan. Presented at *EIC IP6 tracking kick off meeting*, Upton, New York, United States, 2021-03-23 - 2021-03-23. (LA-UR-21-22845)

Li, X. Explore hadronization through heavy flavor probes at the future Electron-Ion Collider. Presented at *INT Electronic Workshop 21-80W, Fragmentation Functions 2021*, Seattle,

Washington, United States, 2021-11-01 - 2021-11-05. (LA-UR-21-30529)

Li, X. Heavy Flavor Physics at the EIC with the ECCE detector. Presented at *The 37th Winter Workshop on Nuclear Dynamics (WWND 2022)*, Puerto Vallarta, Mexico, 2022-02-27 - 2022-03-05. (LA-UR-22-21426)

Li, X. Exploration of matter formation at the next generation collider: the Electron-Ion Collider. Presented at *LANLP Division Cafe*, Los Alamos, New Mexico, United States, 2022-03-10 - 2022-03-10. (LA-UR-22-21953)

Li, X., C. Wong, W. E. Sondheim, J. M. Durham, C. J. Prokop, M. L. Brooks, C. L. Da Silva, A. Morreale and M. X. Liu. Forward silicon tracking detector design and R&D for the future Electron-Ion Collider. Presented at *CPAD 2021*, Stony Brook, New York, United States, 2021-03-18 - 2021-03-22. (LA-UR-21-22558)

Li, X., C. Wong and W. E. Sondheim. Presentations for the 20200022DR 1st year appraisal. . (LA-UR-20-30226)

Li, X., J. M. Durham and C. Wong. LANL open heavy flavor and quarkonia simulation updates for the EIC Yellow Report preparation. Presented at *EIC Pavia online workshop*, Pavia, Italy, 2020-05-20 - 2020-05-22. (LA-UR-20-23799)

Li, X., Y. Corrales Morales, J. M. Durham, M. L. Brooks, W. E. Sondheim, E. L. Renner and C. J. Prokop. Forward silicon vertex/tracking detector design and R&D for the future Electron-Ion Collider. Presented at *APS April Meeting 2022*, New York, New York, United States, 2022-04-09 - 2022-04-12. (LA-UR-22-22526)

Li, X. and A. Morreale. LANL tracking simulation studies for the EIC Yellow Report preparation. Presented at *LANL tracking simulation studies for the EIC Yellow Report preparation*, Philadelphia, Pennsylvania, United States, 2020-03-19 - 2020-03-21. (LA-UR-20-22431)

Li, X. and C. P. Wong. Forward silicon tracker simulation studies in the Fun4All framework. Presented at *The EIC Yellow Report Tracking Working group weekly meeting*, Upton, New York, United States, 2020-05-14 - 2020-05-14. (LA-UR-20-23595)

Li, X. and C. Wong. Open Heavy Flavor and Jet studies for the EIC. Presented at *EIC opportunities for Snowmass*, Stony Brook, New York, United States, 2021-01-25 - 2021-01-29. (LA-UR-21-20714)

Li, X. and J. M. Durham. LANL open heavy flavor and quarkonia simulation studies for the EIC Yellow Report preparation. Presented at *The 1st EIC Yellow Report Workshop at Temple University*, Philadelphia, Pennsylvania, United States, 2020-03-19 - 2020-03-21. (LA-UR-20-22432)

Li, X. and W. E. Sondheim. Collider Experiments Mechanical Support, Vertex Detectors. Presented at *SILICON PIXEL-BASED PARTICLE VERTEX AND TRACKING DETECTORS TOWARDS THE US ELECTRON ION COLLIDER WORKSHOP*, Newport News, Virginia, United States, 2020-09-02 - 2020-09-04. (LA-UR-20-26876)

Morreale, A. Forward Silicon Detector: Layout & performance of LANL 2020022DR. Presented at *Silicon Pixel-based Particle Vertex and Tracking Detectors Towards the US Electron Ion Collider Workshop*, Berkeley, California, United States, 2020-09-02 - 2020-09-04. (LA-UR-20-26997)

Morreale, A. and X. Li. presentation. Presented at *Sant Fe jets workshop*, santa Fe, New Mexico, United States, 2020-02-03 - 2020-02-05. (LA-UR-20-21057)

Saxena, A. B., R. Balakrishnan and R. Dandoloff. Hopfions in Anisotropic Heisenberg Magnets. Presented at *Gaididei Memorial Workshop*, Kiev, Ukraine, 2022-02-02 - 2022-02-02. (LA-UR-22-20781)

Vitev, I. M. DR first year Appraisal. . (LA-UR-20-30048)

Vitev, I. M. Heavy flavor and strangeness in jets and jets +medium. Presented at *DNP Fall Meeting*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-28997)

Vitev, I. M. and X. Li. A new era of nuclear physics at the Electron-Ion Collider. . (LA-UR-20-21116)

Wong, C. Forward Silicon Tracker Design and R&D for the Future Electron-Ion Collider. Presented at *2020 Fall Meeting of the APS Division of Nuclear Physics*, New Orleans, Louisiana, United States, 2020-10-29 - 2020-11-01. (LA-UR-20-28721)

Wong, C. EIC Silicon Tracking in the Forward Direction and Physics Studies. Presented at *Opportunities with heavy flavor at the EIC, CFNS workshop 2020*, Stony Brook, New York, United States, 2020-11-04 - 2020-11-06. (LA-UR-20-29030)

Wong, C. A Forward Silicon Tracker for Heavy Flavors and Jets Measurements in the Future\xc2\xa0Electron-Ion Collider Experiments. Presented at *APS April Meeting 2021*, online, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23495)

Yoon, B. Calculation of Splitting Functions using Machine Learning. . (LA-UR-20-29995)

Yoon, B. In-medium QCD Parton Splitting Functions. . (LA-UR-21-20680)

Yoon, B. In-medium QCD Parton Splitting Functions. . (LA-UR-22-21940)

Posters

Wong, C. A Forward Silicon Tracker for the Future Electron-Ion Collider. Presented at *RHIC & AGS Annual Users' Meeting 2021*, online, New Mexico, United States, 2021-06-08 - 2021-06-11. (LA-UR-21-25323)

High-Gradient, High-Efficiency Radio-frequency (RF) Structures: Smart Design Based on Informed Break-down Suppression

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20200057DR

Project Description

Particle accelerators are established tools for solving national security challenges, as well as for discovery science. Current missions with national security implications include the need to study and develop materials under extreme conditions that never have been accessible before, higher energy accelerators for proton radiography for stockpile stewardship, and improved tools for remote sensing in defense from national security threats. These represent the range of accelerator systems from large to small. The tools and technologies developed in this project will enable follow-on technology development efforts with significant impact on the performance and cost of accelerator systems. Studies on material extremes and proton radiography at increased energies both require large accelerator systems for which new radio-frequency (RF)-structure technology will reduce size (length typically ~ 1000 yards) and complexity, and increase the efficiency of accelerator systems by an order of magnitude. For remote sensing applications the use of such RF-structures provides a path to trailer-bed mountable mobile systems for detection of special nuclear materials (SNM). Novel design and engineering tools will provide the first ever integrated RF-structure design using custom-designed materials that suppress limiting RF-break-down in high performance operation. The effort will also establish the first US-based C-band test accelerator site.

Publications

Journal Articles

Bagchi, S. and D. Perez. Atomistic modeling of the coupling between electric field and bulk plastic deformation in fcc metals. Submitted to *Physical Review Accelerators and Beams*. (LA-UR-21-29271)

Chylek, P., C. Folland, J. Klett and M. K. Dubey. Arctic Amplification and Arctic temperature anomaly: Observed and simulated by thirteen CMIP6 climate models. Submitted to *Quaterly Journal of Royal Meteorological Society*. (LA-UR-21-21658)

Chylek, P., C. Folland, M. K. Dubey and M. Wang. Arctic Amplification 1970-2010: Observed and simulated by CMIP6 climate models. Submitted to *Geophysical Research Letters*. (LA-UR-22-20221)

Schneider, M. E., E. J. Jevarjian, B. Sims, A. M. Altmark and B. Van De Geer. Travelling Wakefield Tube: THz Wakefield Source Powered by Nonrelativistic Electron Beam. Submitted to *Journal of Applied Physics*. (LA-UR-21-26423)

Wang, G., E. I. Simakov and D. Perez. Ab-initio Cu alloy design for high-gradient accelerating structures. Submitted to *Applied Physics Letters*. (LA-UR-22-20039)

Conference Papers

Bagchi, S. and D. Perez. Atomistic modeling of the coupling between electric fields and bulk plastic deformation in RF structures. Presented at *IPAC ' 21*. (Virtual, Brazil, 2021-05-24 - 2021-05-24). (LA-UR-21-24834)

Gorelov, D. V., R. L. Fleming, S. K. Lawrence, D. Perez, M. E. Schneider, M. E. Middendorf, E. I. Simakov and T. Tajima. Status of the C-Band Engineering Research Facility (CERF-NM) Test Stand Development at LANL. Presented at *IPAC'21*. (Campinas, SP, Brazil, 2021-05-24 - 2021-05-28). (LA-UR-21-24879)

I. Lewellen, J. W., D. V. Gorelov, D. Perez, E. I. Simakov and M. E. Schneider. A COUPON TESTER FOR NORMAL CONDUCTING HIGH-GRADIENT MATERIALS. Presented at *12th International Particle Accelerator Conference*. (Campinas, Brazil, 2021-05-24 - 2021-05-24). (LA-UR-21-24740)

Schneider, M. E., R. L. Fleming, E. I. Simakov, D. V. Gorelov, J. W. I. Lewellen, E. Jevarjian and S. Baryshev. FEbreak: A Comprehensive Diagnostic and Automated Conditioning Interface for Breakdown Analysis and Dark Current Effects. Presented at *International particle accelerator conference*. (Campinas, Brazil, 2021-05-24 - 2021-05-28). (LA-UR-21-24789)

Simakov, E. I., D. V. Gorelov, M. E. Middendorf, M. E. Schneider, T. Tajima and M. R. A. Zuboraj. C-band Engineering Test Facility: a New High Gradient Breakdown Test Stand at

LANL. Presented at *International Vacuum Electronics Conference*. (Monterey, California, United States, 2022-04-25 - 2022-04-25). (LA-UR-21-32385)

Simakov, E. I., J. E. Acosta, D. V. Gorelov, T. A. Jankowski, M. F. Kirshner, J. W. I. Lewellen, J. D. Pizzolatto, M. E. Schneider and P. Borchard. DESIGN, FABRICATION, AND COMMISSIONING OF THE MODE LAUNCHERS FOR HIGH GRADIENT C-BAND CAVITY TESTING AT LANL. Presented at *International Particle Accelerator Conference IPAC 2021*. (Campanas, Brazil, 2021-05-24 - 2021-05-24). (LA-UR-21-24878)

Simakov, E. I., R. L. Fleming, D. V. Gorelov, M. F. Kirshner, J. W. I. Lewellen, M. E. Middendorf, M. E. Schneider, T. Tajima, X. Lu, E. Nanni and S. Tantawi. FIRST C-BAND HIGH GRADIENT CAVITY TESTING RESULTS AT LANL. Presented at *International Particle Accelerator Conference IPAC 2021*. (Campinas, Brazil, 2021-05-24 - 2021-05-24). (LA-UR-21-24863)

Books/Chapters

Schneider, M. E. Higher-quality Sources for Electron Accelerators. (LA-UR-21-30750)

Reports

Perez, D. IC report: Materials design for high-gradient RF structures. Unpublished report. (LA-UR-21-21989)

Presentation Slides

Bagchi, S. Atomistic Modeling of the Coupling Between Electric Fields and Bulk Plastic Deformation in Rf Structures. Presented at *IPAC'21*, Virtual, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24725)

Bagchi, S. and D. Perez. Atomistic modeling of the coupling between electric fields and bulk plastic deformation in RF structures. Presented at *International Particle Accelerator Conference 2021*, Campinas, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24425)

Gorelov, D. V., R. L. Fleming, S. K. Lawrence, D. Perez, M. E. Schneider, E. I. Simakov and T. Tajima. Status of the C-Band Engineering Research Facility (CERF-NM) Test Stand Develpment at LANL. Presented at *IPAC'21*, Campinas, SP, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24739)

Gorelov, D. V., R. L. Fleming, S. K. Lawrence, J. W. I. Lewellen, D. Perez, M. E. Schneider, E. I. Simakov and T. Tajima. Status of the C-Band Engineering Research Facility (CERF-NM) Test Stand Develpment at LANL. Presented at *IPAC'21*, Campinas, SP, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24738)

Jevarjian, E. J. Investigating persistent slip markings as breakdown sources by thermal processes. Presented at *Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27550)

Krawczyk, F. L. C-band – The Big Picture. Presented at *LANL 2020 Engineering Capability Review*, Los Alamos, New Mexico, United States, 2020-09-09 - 2020-09-11. (LA-UR-20-26179)

Krawczyk, F. L., E. I. Simakov, D. Perez, G. Wang, A. W. Garmon, M. F. Kirshner, J. T. I. Bradley, E. Nanni, S. Tantawi, D. Gamzina, J. B. Rosenzweig and A. Fukasawa. Technology Development of High-gradient C-band based Accelerators. Presented at *Linear Collider Workshop LCWS 2019*, Sendai, Japan, 2019-10-28 - 2019-11-01. (LA-UR-19-30794)

Lawrence, S. K. Cu Accelerator Part Cleaning. . (LA-UR-21-26214)

I. Lewellen, J. W., D. V. Gorelov, D. Perez, E. I. Simakov and M. E. Schneider. A Coupon Tester for Normal Conducting High-Gradient Materials. Presented at *International Particle Accelerator Conference*, campinas, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24614)

I. Lewellen, J. W., D. V. Gorelov, D. Perez and E. I. Simakov. High-gradient C-band research at Los Alamos. Presented at *International Workshop on Breakdown Science and High Gradient Technology (HG2021)*, los alamos, New Mexico, United States, 2021-04-19 - 2021-04-21. (LA-UR-21-23725)

I. Lewellen, J. W., E. I. Simakov, T. Tajima and P. Pizzol. Status of Cryo Work at LANL. . (LA-UR-21-21926)

Perez, D. C-Band materials modeling efforts at LANL. . (LA-UR-20-28389)

Perez, D. Atomistic modeling of the coupling between electric fields and bulk plastic deformation in RF structures. Presented at *High Gradient 2021*, Stanford, California, United States, 2021-04-19 - 2021-04-19. (LA-UR-21-24553)

Perez, D. IC Project w20_cband FY21 highlight. . (LA-UR-22-21649)

Schneider, M. E. Field Emission Electron Sources for Ultra Bright Beam Compact Accelerators. Presented at *SLAC Colloquium series*, menlo park, California, United States, 2021-11-10 - 2021-11-10. (LA-UR-21-30940)

Schneider, M. E., B. Sims, E. J. Jevarjian, B. van der Geer, A. Altmark and S. Baryshev. THz Wakefield Source Powered by Nonrelativistic Electron Beams. Presented at *Pulsed Power Conference*, Denver, Colorado, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-30866)

Schneider, M. E., B. Sims, E. J. Jevarjian, R. Shinohara, T. Nikhar, T. Posos, W. Lui, J. Power and S. Baryshev. Bright Beam Ampere Class (N)UNCD Field Emission Cathode for RF Guns. Presented at *AccApp21*, DC, District Of Columbia, United States, 2021-11-30 - 2021-12-04. (LA-UR-21-30876)

Schneider, M. E., B. Sims, E. J. Jevarjian, R. Shinohara, T. Nikhar, T. Posos, W. Lui, S. Baryshev, j. Power and J. Shoa. Bright Beam Ampere Class (N)UNCD Field Emission Cathode for RF Guns. Presented at *pulsed power Conference*, Denver, Colorado, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-30865)

Schneider, M. E., B. sims, E. J. Jevarjian, A. Altmark, B. Van der Geer and S. Baryshev. Forensic Applications for THz

Wakefield Source Powered by Nonrelativistic Electron Beams. Presented at *AccApp 21*, DC, District Of Columbia, United States, 2021-11-30 - 2021-12-04. (LA-UR-21-30868)

Schneider, M. E., E. Jevarjian, J. Shao, T. Posos, T. Nikhar, W. Lui and S. V. Baryshev. Demonstration of Ampere-class Field Emission Cathodes Operating at 100 MV/M and Excess of Child-Langmuir Law. Presented at *Advanced accelerator concepts 2020: seminar series*, online, California, United States, 2021-01-13 - 2021-01-13. (LA-UR-21-20177)

Schneider, M. E., E. Jevarjian, J. Shao and S. Baryshev. FEbeam: A Comprehensive Field Emission Data Processing for Field Emission and Breakdown Analysis in RF Environment. Presented at *International particle accelerator conference*, Campinas, Brazil, 2021-06-24 - 2021-06-28. (LA-UR-21-24610)

Schneider, M. E., E. Jevarjian, J. Shao and S. V. Baryshev. FEbeam: A Comprehensive Field Emission Data Processing for Field Emission and Breakdown Analysis in RF Environment. Presented at *9th International Workshop on Mechanisms of Vacuum Arcs (MeVArc 2021)*, online, Switzerland, 2021-03-08 - 2021-03-12. (LA-UR-21-22291)

Schneider, M. E., E. Jevarjian and S. Baryshev. A Field Emission Initial Particle Distribution Freeware for Advanced Beam Dynamics Simulations Based on Fowler- Nordheim Equations for High Gradient Accelerators. Presented at *International particle accelerator conference*, Campinas, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24612)

Schneider, M. E., H. L. Andrews, D. Kim, K. Nichols, M. T. Pettes, E. I. Simakov, E. J. Jevarjian, T. Posos, S. Baryshev, J. Power and J. Shoa. Pattern Beam Production from Diamond Field Emitter Arrays (DFEAs). Presented at *AccApp 21*, DC, District Of Columbia, United States, 2021-11-30 - 2021-12-04. (LA-UR-21-30875)

Schneider, M. E., J. W. I. Lewellen, E. I. Simakov, D. V. Gorelov, R. L. Fleming, S. V. Baryshev and E. Jevarjian. FEbreak: A Comprehensive Diagnostic and Automated Conditioning Interface for Analysis of Breakdown and Dark Current Effects. Presented at *International particle accelerator conference*, Campinas, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24615)

Schneider, M. E., R. L. Fleming, E. Jevarjian, E. I. Simakov, S. V. Baryshev, D. V. Gorelov and J. W. I. Lewellen. FEbreak: A Comprehensive Diagnostic and Automated Conditioning Interface for Analysis of Breakdown and Dark Current Effects. Presented at *9th International Workshop on Mechanisms of Vacuum Arcs (MeVArc 2021)*, online, Switzerland, 2021-03-08 - 2021-03-12. (LA-UR-21-22292)

Simakov, E. I. New accelerator capabilities with the high-gradient C-band. . (LA-UR-21-30757)

Simakov, E. I., J. E. Acosta, A. N. Black, A. G. Glover, D. V. Gorelov, T. A. Jankowski, J. W. I. Lewellen, S. K. Lawrence, J. D. Pizzolatto and M. E. Schneider. Development and high power testing of C-band accelerator components. Presented at *International Workshop on Breakdown Science and High Gradient Technology HG2021*, Menlo Park, California, United States, 2021-04-19 - 2021-04-19. (LA-UR-21-23724)

Simakov, E. I., J. E. Acosta, D. V. Gorelov, T. A. Jankowski, M. F. Kirshner, J. W. I. Lewellen, J. D. Pizzolatto and M. E. Schneider. Design, fabrication, and commissioning of the mode launchers for high gradient C-band cavity testing at LANL. Presented at *International Particle Accelerator Conference IPAC 2021*, Campinas, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24743)

Simakov, E. I., J. E. Acosta, D. V. Gorelov, T. A. Jankowski, M. F. Kirshner, J. W. I. Lewellen, J. D. Pizzolatto and M. E. Schneider. Design, fabrication, and commissioning of the mode launchers for high gradient C-band cavity testing at LANL. Presented at *International Particle Accelerator Conference IPAC 2021*, Campinos, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24744)

Simakov, E. I., R. L. Fleming, D. V. Gorelov, M. F. Kirshner, J. W. I. Lewellen, M. E. Middendorf, M. E. Schneider, T. Tajima, X. Lu, E. Nanni and S. Tantawi. First C-band high gradient cavity testing results at LANL. Presented at *International Particle Accelerator Conference IPAC 2021*, Campinas, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24742)

Simakov, E. I., R. L. Fleming, D. V. Gorelov, M. F. Kirshner, J. W. I. Lewellen, M. E. Middendorf, M. E. Schneider, T. Tajima, X. Xu, E. Nanni and S. Tantawi. First C-band high gradient cavity testing results at LANL. Presented at *International Particle Accelerator Conference IPAC 2021*, Campinas, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24741)

Simakov, E. I., R. L. Fleming, D. V. Gorelov, M. F. Kirshner, J. W. I. Lewellen, M. E. Middendorf, P. Pizzol, M. E. Schneider and T. Tajima. UC XFEL Testing Capabilities at LANL. Presented at *Towards an Ultra-Compact X-ray Free-Electron Laser*, Los Angeles, California, United States, 2021-07-19 - 2021-07-19. (LA-UR-21-26871)

Wang, G. and D. Perez. Ab-initio alloy design for C-band accelerators. Presented at *International Workshop on Breakdown Science and High Gradient Technology (HG2021)*, Los Alamos, New Mexico, United States, 2021-04-19 - 2021-04-21. (LA-UR-21-23694)

Posters

Bagchi, S. and D. Perez. Scale Bridging Molecular Dynamics to Couple Electric Fields with Plastic Deformation in FCC Metals. Presented at *Society of Engineering Sciences (SES) 2021 Virtual Conference*, Virtual, New Mexico, United States, 2021-09-15 - 2021-09-15. (LA-UR-21-29362)

Simakov, E. I. AFEL Layout. Presented at *Future US Colliders Workshop*, Menlo Park, California, United States, 2022-01-18 - 2022-01-18. (LA-UR-22-20501)

Predictive Understanding of Device Performance Through Innovative Measurement, Modeling, and Simulation on Radiochemical Dosimeters (U)

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20200108DR

Project Description

Radiochemical diagnostics (aka "radchem") have been a crucial ingredient of nuclear weapons testing since inception, and efforts continue to this day to increase their usefulness and predictive capability. We will develop a novel, innovative technique to greatly reduce uncertainties for key radchem nuclear reaction rates, thereby enabling much more predictive understanding of nuclear weapons. Almost none of these rates have been measured and so they are very uncertain. Our main goal is to solve this problem by developing the first technique capable of determining key nuclear reaction rates with the required accuracy. Once demonstrated, this capability can be applied to many more cases of high interest to radchem as well as technical nuclear forensics and nuclear astrophysics, thus impacting additional Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions.

Publications

Journal Articles

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. New capability for neutron transmission measurements at LANSCE: The DICER instrument. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-21-29960)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. New apparatus for neutron capture measurements on extra small radioactive samples: The DICER instrument at LANSCE. Submitted to *Neutron News*. (LA-UR-22-21702)

Stamatopoulos, A., P. E. Koehler, A. Matyskin, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. New capability for indirect neutron capture measurements: The DICER instrument at LANSCE. 2022. *EPJ Web of Conferences*. **260**: 03006. (LA-UR-21-31697 DOI: 10.1051/epjconf/202226003006)

Conference Papers

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. A new approach for indirect capture measurements:The DICER neutron transmission station at LANSCE. Presented at *Hellenic Nuclear Physic Society Symposium 2021 (HNPS2021)*. (Athens, Greece, 2021-09-24 - 2021-09-25). (LA-UR-21-32022)

Presentation Slides

DiGiovine, B. J. Enabling direct reaction studies with small, highly radioactive samples. Presented at *Workshop for Applied Nuclear Data Activities 2022*, Cisco WebEx (Virtually), New Mexico, United States, 2022-02-28 - 2022-02-04. (LA-UR-22-21560)

Erjavec, T., J. L. Ullmann and P. E. Koehler. ARTIE: Measuring the 57keV neutron cross-section of liquid argon. Presented at *APS Far West Section (remote)*, Davis, California, United States, 2020-10-10 - 2020-10-10. (LA-UR-20-30192)

Koehler, P. E. DICER (Device for Indirect Capture Experiments on Radionuclides). Presented at *Nuclear Data Advisory Group*, santa fe, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21109)

Koehler, P. E., T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, J. M. O'Donnell, R. Reifarth, G. Y. Rusev, A. Stamatopoulos and J. L. Ullmann. 149Sm Results from DICER Plus DANCE. Presented at *Nuclear Data Advisory Group*, new york, New York, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31180)

Koehler, P. E., T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, J. M. O'Donnell, R. Reifarth, G. Y. Rusev, A. Stamatopoulos and J. L. Ullmann. DICER, The Newest LANSCE Nuclear Physics Instrument. Presented at *Neutrons in Science, Technology and Applications*, Geneva, Switzerland, 2021-11-22 - 2021-11-22. (LA-UR-21-31377)

Pagani, L., S. Andringa, Y. Bezawada, T. Erjavec, J. He, J. Huang, P. E. Koehler, M. J. Mocko, M. Mulhearn, E. Pantic, L. Pickard, R. Svoboda, J. L. Ullmann and J. Wang. ARTIE (near)-final results. Presented at *DUNE collaboration*

meeting (remote), none, California, United States, 2020-09-23 - 2020-09-23. (LA-UR-20-29932)

Rusev, G. Y., P. E. Koehler, A. Stamatopoulos, A. J. Couture, B. J. DiGiovine and J. L. Ullmann. First DICER results from 191Ir and 193Ir. Presented at *LDRD DR Project Appraisal (20200108DR Koehler)*, Los Alamos, New Mexico, United States, 2020-12-10 - 2020-12-10. (LA-UR-20-30110)

Stamatopoulos, A., P. E. Koehler, A. J. Couture, B. J. DiGiovine, G. Y. Rusev and J. L. Ullmann. A new approach for indirect capture measurements: The DICER neutron transmission station at LANSCE. Presented at *HNPS2021*, Athens, Greece, 2021-09-24 - 2021-09-25. (LA-UR-21-29104)

Stamatopoulos, A., P. E. Koehler, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. New capability for indirect neutron capture measurements: The DICER instrument at LANSCE. Presented at *Nuclei in the Cosmos 2021*, Chengdu, China, 2021-09-21 - 2021-09-25. (LA-UR-21-29183)

Stamatopoulos, A., P. E. Koehler, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. A new apparatus for indirect neutron capture measurements at LANSCE. Presented at *2021 Fall Meeting of the APS Division of Nuclear Physics*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-14. (LA-UR-21-29963)

Posters

Stamatopoulos, A., P. E. Koehler, E. M. Bond, T. A. Bredeweg, A. J. Couture, B. J. DiGiovine, M. E. Fassbender, A. C. Hayes-Sterbenz, A. L. Keksis, A. Matyskin, D. K. Parsons, G. Y. Rusev, J. L. Ullmann and C. Vermeulen. DICER: A new Device for Indirect Capture Experiments on Radionuclides. Presented at *African Nuclear Physics Conference 2021*, Online, South Africa, 2021-09-20 - 2021-09-24. (LA-UR-21-28849)

Revolutionary Advances in Nuclear Data to Underpin LANL 21st Century Missions

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Project Description

Nuclear data and simulation advancements are important to the Los Alamos National Laboratory (LANL) mission. The work in the EUCLID (Experiments Underpinned by Computational Learning for Improvements in nuclear Data) project is an important step towards long-term mission needs. One major goal of EUCLID is to reduce compensating errors in nuclear data that impede our predictive capabilities. This first-of-a-kind capability builds upon renowned LANL strengths in nuclear-data evaluation, transport codes, validation experiments, and machine learning. If successful, the advancements of this work will have cross-cutting impact which can be applied to answer urgent mission needs representing national security challenges for the Laboratory's Plutonium Facility (PF-4) pit production, Design for Manufacturing, Enhanced Capabilities for Subcritical Experiments (ECSE), Weapons and global security assessments, and micro-reactor design.

Publications

Journal Articles

Herman, M. W., D. A. Brown, R. Capote, M. B. Chadwick, W. Haeck, J. D. Hutchinson, T. Kawano, D. Neudecker, G. Palmiotti, M. Salvatores, P. Talou, A. Trkov and M. C. White. Infrastructure for the new paradigm of nuclear reaction evaluation. Submitted to *Annals of Nuclear Energy*. (LA-UR-21-21303)

Kolos, K., V. Sobes, R. Vogt, C. Romano, M. Smith, L. Bernstein, D. A. Brown, M. Burkey, Y. Danon, M. Elsawi, B. Goldblum, L. Heilbronn, S. Hogle, J. D. Hutchinson, B. Loer, E. McCutchan, M. R. Mumpower, E. M. O'Brien, C. Percher, P. Peplowski, J. Ressler, N. Schunck, N. W. Thompson, A. Voyles, W. Wieselquist and M. Zerkle. Current Nuclear Data Needs for Applications. Submitted to *Physical Review Research*. (LA-UR-21-29987)

*Neudecker, D., O. Cabellos, A. R. Clark, M. J. Grosskopf, W. Haeck, M. W. Herman, J. Hutchinson, T. Kawano, A. E. Lovell, I. Stetcu, P. Talou and S. Vander Wiel. Informing nuclear physics via machine learning methods with differential and integral experiments. 2021. *Physical Review C*. **104** (3): 034611. (LA-UR-21-22465 DOI: 10.1103/PhysRevC.104.034611)

Neudecker, D., O. Cabellos, A. R. Clark, W. Haeck, R. Capote, A. Trkov, M. C. White and M. E. Rising. Which nuclear data can be validated with LLNL pulsed-sphere experiments. Submitted to *Annals of Nuclear Energy*. (LA-UR-20-28636)

Conference Papers

Alwin, J. L., J. D. Hutchinson, N. A. Kleedtke, A. R. Clark, T. E. Cutler, W. Haeck, R. C. Little, D. Neudecker, M. E. Rising, T. A. Smith and N. W. Thompson. Investigating Fission Reaction Rate Ratio Sensitivities. Presented at *American Nuclear Society (ANS) Nuclear Criticality Safety Division (NCSD) Topical Meeting*. (Anaheim, California, United States, 2022-06-12 - 2022-06-12). (LA-UR-22-20792)

Cutler, T. E., J. D. Hutchinson, D. Neudecker, W. Haeck, A. R. Clark and M. E. Rising. Reactivity Coefficient Measurements and Sensitivity Studies. Presented at *American Nuclear Society (ANS) Nuclear Criticality Safety Division (NCSD) Topical Meeting*. (Anaheim, California, United States, 2022-06-12 - 2022-06-12). (LA-UR-22-20850)

Cutler, T. E., J. D. Hutchinson, N. A. Kleedtke, M. E. Rising, D. Neudecker, R. C. Little and N. W. Thompson. Validation of Jezebel Reactivity Coefficients and Sensitivity Analysis. Presented at *2021 ANS Winter Meeting*. (Washington, District Of Columbia, United States, 2021-11-30 - 2021-11-30). (LA-UR-21-26475)

Hutchinson, J. D., A. R. Clark, N. A. Kleedtke, M. E. Rising, R. G. Sanchez and R. A. J. Weldon. Equivalent Fundamental-Mode Source Simulations for Spherical Uranium and Plutonium Systems. Presented at *American Nuclear Society (ANS) Nuclear Criticality Safety Division (NCSD) Topical Meeting*. (Anaheim, California, United States, 2022-06-13 - 2022-06-13). (LA-UR-22-20752)

Hutchinson, J. D., N. A. Kleedtke, J. L. Alwin, A. R. Clark, T. E. Cutler, W. Haeck, R. C. Little, D. Neudecker, M. E. Rising, T. A. Smith and N. W. Thompson. Investigation of Delayed Neutron Sensitivities for Several ICSBEP Benchmarks using MCNP. Presented at *American Nuclear Society Winter Meeting*. (Washington DC, District Of Columbia, United States, 2021-11-30 - 2021-11-30). (LA-UR-21-26405)

Kleedtke, N. A., J. D. Hutchinson, M. Y. Hua and M. E. Rising. Sensitivity Coefficients Calculated for the Prompt Neutron Decay Constant At or Near Delayed Critical. Presented at *American Nuclear Society (ANS) Annual Meeting*. (Anaheim, California, United States, 2022-06-12 - 2022-06-16). (LA-UR-22-20775)

Lamproe, J. R., T. E. Cutler, M. Y. Hua, A. R. Clark, J. D. Hutchinson, S. D. Clarke and S. Pozzi. A Verification of Flux Sensitivity Estimates Using the MCNP Tally Perturbation Tool. Presented at *2021 ANS Winter Meeting and Technology Expo*. (Washington, District Of Columbia, United States, 2021-11-30 - 2021-12-04). (LA-UR-21-26595)

Lewis, A., D. Neudecker, A. Koning and M. Fleming. SG50 Data-format Requirement Document for an Automatically Readable, Comprehensive and Curated Experimental Reaction Database. Presented at *WPEC SG 50*. (Paris, France, 2020-11-12 - 2020-11-12). (LA-UR-20-28933)

Reports

Alwin, J. L., A. R. Clark, T. E. Cutler, M. J. Grosskopf, W. Haeck, M. W. Herman, J. D. Hutchinson, N. A. Kleedtke, J. R. Lamproe, R. C. Little, I. J. Michaud, D. Neudecker, M. E. Rising, T. A. Smith, N. W. Thompson and S. A. Vander Wiel. EUCLID Sensitivity Database. Unpublished report. (LA-UR-22-21534)

Cabellos, O. and D. Neudecker. Machine Learning in Nuclear Science and Engineering Applications. Unpublished report. (LA-UR-21-28449)

Neudecker, D. Short Summaries of Talks for the IAEA INDEN Meeting and IAEA Consultancy Meeting on Machine Learning for Nuclear Data. Unpublished report. (LA-UR-20-30057)

Neudecker, D. Test Results for Checking Reliability of Selected ENDF/B-VIII.0 Evaluated Uncertainties. Unpublished report. (LA-UR-22-21551)

Neudecker, D., N. Dwivedi, E. Alhassan and G. Schnabel. MACHINE LEARNING FOR NUCLEAR DATA. Unpublished report. (LA-UR-21-29983)

Presentation Slides

Alwin, J. L., A. R. Clark, T. E. Cutler, W. Haeck, J. D. Hutchinson, N. A. Kleedtke, D. Neudecker and M. E. Rising. The EUCLID Sensitivity Library. Presented at *WPEC SG-46*, Paris, France, 2022-03-15 - 2022-03-15. (LA-UR-22-21896)

Clark, A. R. Overview of dissertation and postdoctoral research. . (LA-UR-21-20860)

Clark, A. R. Optimal experiment design and nuclear data validation with diverse benchmarks. Presented at *Nuclear Criticality Safety Program Technical Review Meeting*, Online, New Mexico, United States, 2021-02-23 - 2021-02-25. (LA-UR-21-21446)

Clark, A. R. Impact of nuclear data validation with uncertainty quantification and diverse benchmarks on criticality safety. . (LA-UR-21-22043)

Cutler, T. E., J. D. Hutchinson, N. A. Kleedtke, M. E. Rising, D. Neudecker, R. C. Little and N. W. Thompson. Validation of Jezebel Reactivity Coefficients and Sensitivity Analysis. Presented at *ANS 2021 Winter Meeting*, Washington, District Of Columbia, United States, 2021-11-30 - 2021-11-30. (LA-UR-21-31637)

Grosskopf, M. J. Using Machine Learning to Explore, Diagnose, and Correct for Bias in Nuclear Data. Presented at *IAEA Consultancy Meeting on Machine Learning for Nuclear Data*, Online, New Mexico, United States, 2020-12-07 - 2020-12-11. (LA-UR-20-30054)

Haeck, W., A. R. Clark and M. W. Herman. Calculating the impact of nuclear data changes with Crater. Presented at *ANS Winter Meeting*, Chicago, Illinois, United States, 2020-11-16 - 2020-11-20. (LA-UR-20-29434)

Hutchinson, J. D., D. Neudecker, M. J. Grosskopf, J. L. Alwin, A. R. Clark, T. E. Cutler, N. A. Gibson, W. Haeck, M. W. Herman, N. A. Kleedtke, I. J. Michaud, M. E. Rising, T. A. Smith, N. W. Thompson, S. A. Vander Wiel and R. C. Little. Identifying unconstrained physics spaces in nuclear data and resolving them via integral experiments. . (LA-UR-21-25625)

Hutchinson, J. D., J. L. Alwin, A. R. Clark, T. E. Cutler, M. J. Grosskopf, W. Haeck, M. W. Herman, N. A. Kleedtke, J. R. Lamproe, R. C. Little, I. J. Michaud, D. Neudecker, M. E. Rising, T. A. Smith, N. W. Thompson and S. A. Vander Wiel. Getting sensitivities for various integral responses supporting nuclear data validation and adjustment. Presented at *CSEWG 2021*, New York, New York, United States, 2021-11-15 - 2021-11-19. (LA-UR-21-31279)

Hutchinson, J. D., J. L. Alwin, A. R. Clark, T. E. Cutler, M. J. Grosskopf, W. Haeck, M. W. Herman, N. A. Kleedtke, J. R. Lamproe, R. C. Little, I. J. Michaud, D. Neudecker, M. E. Rising, T. A. Smith, N. W. Thompson and S. A. Vander Wiel. EUCLID: Experiments Underpinned by Computational Learning for Improvements in nuclear Data. Presented at *Nuclear Criticality Safety Program (NCSP) Technical Program Review*, Oak Ridge, Tennessee, United States, 2022-02-16 - 2022-02-16. (LA-UR-22-21097)

Hutchinson, J. D., J. L. Alwin, A. R. Clark, T. E. Cutler, M. J. Grosskopf, W. Haeck, M. W. Herman, N. A. Kleedtke, J. R. Lamproe, R. C. Little, I. J. Michaud, D. Neudecker, M. E. Rising, T. A. Smith, N. W. Thompson and S. A. Vander Wiel. EUCLID adjustment including multiple integral responses. Presented at *Workshop for Applied Nuclear Data Activities*, Washington DC, District Of Columbia, United States, 2022-03-01 - 2022-03-01. (LA-UR-22-21290)

Hutchinson, J. D., J. L. Alwin, T. J. Grove, N. A. Kleedtke, I. J. Michaud, M. E. Rising, T. A. Smith, N. W. Thompson and R. C. Little. Sensitivity Studies, Gap Analysis, and Benchmark Experiment Optimization for Reactor Physics and Criticality Safety Applications. Presented at *ANS Winter Meeting*,

Chicago, Illinois, United States, 2020-11-16 - 2020-11-16. (LA-UR-20-29405)

Hutchinson, J. D., N. A. Kleedtke, J. L. Alwin, T. E. Cutler, W. Haeck, A. R. Clark, R. C. Little, D. Neudecker, M. E. Rising, T. A. Smith and N. W. Thompson. Investigation of Delayed Neutron Sensitivities for Several ICSBEP Benchmarks using MCNP. Presented at *American Nuclear Society Winter Meeting*, Washington, District Of Columbia, United States, 2021-11-29 - 2021-11-29. (LA-UR-21-31592)

Kleedtke, N. A., I. J. Michaud, M. E. Rising, T. J. Grove, J. D. Hutchinson and B. C. Kiedrowski. Gaussian Process Optimization of Sensitivity-Based Similarity Metrics between New Nuclear Applications and New/Existing Benchmarks. Presented at *American Nuclear Society Virtual Winter Meeting*, Chicago, Illinois, United States, 2020-11-16 - 2020-11-19. (LA-UR-20-29409)

Kleedtke, N. A., J. D. Hutchinson, I. J. Michaud and T. J. Grove. Effective Delayed Neutron Fraction and Reactivity Coefficient Sensitivity-based Similarity Metrics for New Experiment Design Optimization. Presented at *2021 ANS Winter Meeting and Technology Expo*, Washington, District Of Columbia, United States, 2021-11-30 - 2021-12-03. (LA-UR-21-31657)

Lamproe, J. R., T. E. Cutler, M. Y. Hua, A. R. Clark, J. D. Hutchinson, S. D. Clarke and S. A. Pozzi. A Verification of Flux Sensitivity Estimates Using the MCNP Tally Perturbation Tool. Presented at *American Nuclear Society (ANS) Winter Conference*, Washington, District Of Columbia, United States, 2021-11-30 - 2021-12-03. (LA-UR-21-31638)

Michaud, I. J., N. A. Kleedtke and J. D. Hutchinson. Bayesian Optimization and MCNP. Presented at *MCNP Symposium 2021*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26776)

Neudecker, D. Using Machine Learning Algorithms for Large-scale Nuclear-data Validation.. Presented at *Student seminar*, Madrid, Spain, 2020-10-26 - 2020-10-26. (LA-UR-20-28240)

Neudecker, D. Validating Nuclear Data Augmented by Random Forests. Presented at *IAEA Consultancy Meeting on Machine Learning for Nuclear Data*, VIenna, Austria, 2020-12-08 - 2020-12-11. (LA-UR-20-29856)

Neudecker, D. Slides for the WANDA session on "Expanded Benchmarks & Validation for Nuclear Data". Presented at *WANDA2021*, Washington, District Of Columbia, United States, 2021-01-25 - 2021-02-03. (LA-UR-21-20322)

Neudecker, D. Example on how to (intelligently) augment the nuclear-data pipeline with machine learning. Presented at *WANDA2021*, Washington, District Of Columbia, United States, 2021-01-25 - 2021-02-03. (LA-UR-21-20366)

Neudecker, D. Using Machine Learning Algorithms for Large-scale Nuclear-data Validation. Presented at *\xc2\xa03rd Workshop of Spanish Users on Nuclear Data on\xc2\xa0 "Machine Learning in Nuclear Science and Technology Applications"\xc2\xa0*, Madrid, Spain, 2021-05-27 - 2021-05-27. (LA-UR-21-24921)

Neudecker, D. Using MCNP-calculated sensitivities and machine learning to identify unconstrained physics spaces in nuclear data. Presented at *2021 MCNP\xc2\xae User Symposium*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26267)

Neudecker, D. Identifying Unconstrained Physics Spaces in Nuclear Data by Applying ML to Heterogeneous and Intertwined data. Presented at *AI for Atoms*, Vienna, Austria, 2021-10-25 - 2021-10-29. (LA-UR-21-30360)

Neudecker, D. Large-scale Nuclear-data Validation of ENDF/B-VIII.0 Supported by ML, Sensitivity Analysis and Differential Information. Presented at *INDEN*, Vienna, Austria, 2021-11-01 - 2021-11-05. (LA-UR-21-30900)

Neudecker, D. Using ML and various integral responses to identify unconstrained physics spaces in nuclear data. Presented at *Nuclear Data Week*, Paris, France, 2021-11-22 - 2021-11-26. (LA-UR-21-31423)

Neudecker, D. What now: we can identify measurement needs for nuclear data, but how do we reliably resolve these currently unconstrained physics spaces?. Presented at *ISNET*, East Lansing, Michigan, United States, 2021-12-13 - 2021-12-16. (LA-UR-21-32066)

Neudecker, D. Context of Adjustment & Session Overview. Presented at *WANDA*, Los Alamos, New Mexico, United States, 2022-02-28 - 2022-03-04. (LA-UR-22-21321)

Neudecker, D., A. Lewis, R. Casperson and P. Talou. "Nuclear Data Adjustments and Impact to Applications" at WANDA2022. Presented at *CSEWG 2021*, New York, New York, United States, 2021-11-15 - 2021-11-19. (LA-UR-21-31429)

Neudecker, D., A. Lewis, R. Casperson and P. Talou. Nuclear Data Adjustment and Impact on Applications. Presented at *WANDA*, Washington, District Of Columbia, United States, 2022-03-04 - 2022-03-04. (LA-UR-22-22054)

Rising, M. E. Sensitivity Tool Needs for Modern Nuclear Data Validation. Presented at *Workshop for Applied Nuclear Data Activities (WANDA 2021)*, Cisco WebEx (Virtually), New Mexico, United States, 2021-01-25 - 2021-02-03. (LA-UR-21-20511)

Rising, M. E. Whisper Use of Nuclear Data Covariances. Presented at *2021 Virtual Mini-CSEWG Meeting*, Online, New Mexico, United States, 2021-08-16 - 2021-08-19. (LA-UR-21-28292)

Rising, M. E., T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, R. A. I. Forster, C. J. Josey, J. A. Kulesza, A. J. Zukaitis, J. E. Sweezy, S. Swaminarayan and L. Casswell. Recent MCNP6(R) Code Developments and Improvements for Nuclear Engineering Applications. Presented at *2021 Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25703)

Rising, M. E. and A. R. Clark. Prototype of a New Fixed-source Sensitivity Tally Capability. Presented at *2021 MCNP(R) User Symposium*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26810)

Thompson, N. W., M. E. Rising, D. Neudecker, J. D. Hutchinson, A. C. I. Kahler, A. R. Clark, M. W. Herman, J. L. Alwin, M. J. Grosskopf, W. Haeck, S. A. Vander Wiel and T. E. Cutler. Questionable Benchmarks. Presented at *WPNCS SG-8*, Paris, France, 2021-07-05 - 2021-07-09. (LA-UR-21-26262)

Vander Wiel, S. A., D. C. Francom and B. P. Weaver. Propagating Uncertain Functional Inputs Through Neutronics Simulations. Presented at *Symposium on Data Science and Statistics*, Online, New Mexico, United States, 2021-06-02 - 2021-06-04. (LA-UR-21-25942)

Posters

Lamproe, J. R., T. E. Cutler, M. Y. Hua, A. R. Clark, J. D. Hutchinson, M. E. Rising, S. D. Clarke and S. Pozzi. Verification of Upcoming MCNP Features For Estimating Nuclear Data Sensitivities in Fixed Source Simulation. Presented at *MTV Workshop*, Ann Arbor, Michigan, United States, 2022-03-21 - 2022-03-23. (LA-UR-22-22512)

Lamproe, J. R., T. E. Cutler, M. Y. Hua, J. D. Hutchinson and S. Pozzi. Validation of Nuclear Data Sensitivity Calculations by the MCNP PERT Card. Presented at *2021 MTV Virtual Workshop*, Ann Arbor, Michigan, United States, 2021-03-29 - 2021-03-31. (LA-UR-21-22734)

Thompson, N. W., T. E. Cutler, J. D. Hutchinson, D. Neudecker and H. R. Trellue. Nuclear Data in Support of Reactor Development. . (LA-UR-21-25034)

Beyond the Standard Model through Precision Neutron Decay

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Project Description

The standard model of particle physics is an extremely successful theory that describes the interactions of subatomic particles, however the theory appears to be incomplete as it does not predict some of the fundamental observed properties of the universe, such as the predominance of matter over antimatter. Modifications to the standard model theory can explain these observations, while also implying the existence of new subatomic particles. This project aims to test the standard model at very high precision through measurement of the radioactive decay of the neutron, which could reveal the presence of additional subatomic particles or otherwise provide stringent constraints on new theories. The neutron is a constituent of the atomic nuclei of everyday matter. When free from an atomic nucleus, the neutron is unstable and decays after an average of 15 minutes into a proton, electron and antineutrino. This project will develop experiments to improve measurements of two properties of neutron decay, perform state-of-the-art theoretical calculations to interpret results in terms of the standard model, and evaluate constraints on beyond standard model theories. This effort is well-aligned with the Department of Energy (DOE)-Office of Science goal of determining the new standard model of particle physics.

Publications

Journal Articles

A. L. *. d. V. J. *. M. E. *. O. F. Dekens, W. *. and E. Mereghetti. A low-energy perspective on the minimal left-right symmetric model. 2021. *Journal of High Energy Physics*. **2021** (11): 127. (LA-UR-21-26789 DOI: 10.1007/JHEP11(2021)127)

Gonzalez, F. M., E. M. Fries, C. Cude-Woods, T. Bailey, M. Blatnik, L. J. Broussard, N. B. Callahan, J. H. Choi, S. M. Clayton, S. A. Currie, M. Dawid, E. B. Dees, B. W. Filippone, W. Fox, P. Geltenbort, E. George, L. Hayen, K. P. Hickerson, M. A. Hoffbauer, k. Hoffman, A. Holley, T. M. Ito, A. Komives, C. Y. Liu, M. Makela, C. L. Morris, R. Musedinovic, C. O'Shaughnessy, R. W. J. Pattie, J. Ramsey,

D. J. Salvat, A. Saunders, E. Sharapov, S. A. Slutsky, V. Su, X. Sun, C. Swank, Z. Tang, W. Uhrich, J. Vanderwerp, P. Walstrom, Z. Wang, W. Wei and A. R. Young. A high-precision measurement of the neutron lifetime with UCN. Submitted to *Physical Review Letters*. (LA-UR-21-24910)

Gupta, R., M. Hoferichter, E. Mereghetti, B. Yoon, T. Bhattacharya and S. Park. The nucleon sigma term from lattice QCD. Submitted to *Physical Review Letters*. (LA-UR-21-24759)

Gupta, R., b. Joo, T. Bhattacharya, B. Yoon, S. Park, S. Mondal, F. winter and Y. C. Jang. Precision Nucleon Charges and Form Factors Using 2+1-flavor Lattice QCD. Submitted to *Physical Review D*. (LA-UR-21-20526)

Mereghetti, E., G. King, A. Baroni, V. Cirigliano, S. Gandolfi, L. Hayen, S. Pastore and M. Piarulli. Ab initio calculation of the beta decay spectrum of 6He. Submitted to *Physical Review C*. (LA-UR-21-31938)

Mereghetti, E., R. Boughezal and F. Petriello. Dilepton production in the SMEFT at O(1/Lambda^4). Submitted to *Journal of High Energy Physics*. (LA-UR-21-25379)

Morris, C., J. O. Perry and F. E. Merrill. Cosmic ray radiography of a human phantom. Submitted to *Radiography*. (LA-UR-21-24872)

*Wang, Z., K. Kuk, C. B. Cude-Woods, C. R. Chavez, J. H. Choi, J. Estrada, M. A. Hoffbauer, S. E. Holland, M. F. Makela, C. Morris, E. Ramberg, E. R. Adamek, T. Bailey, M. Blatnik, L. J. Broussard, M. A. Brown, N. B. Callahan, S. Clayton, S. A. Currie, B. W. Filippone, E. M. Fries, P. Geltenbort, F. Gonzalez, M. T. Hassan, L. Hayen, K. P. Hickerson, A. T. Holley, T. Ito, C. Y. Liu, P. Merkel, R. Musedinovic, C. M. O'Shaughnessy, R. W. J. Pattie, B. Plaster, D. J. Salvat, A. Saunders, E. I. Sharapov, X. Sun, Z. Tang, W. Wei, J. W. Wexler and A. R. Young. Projection imaging with ultracold neutrons. 2021. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. 165306. (LA-UR-21-21480 DOI: 10.1016/j.nima.2021.165306)

Conference Papers

Gupta, R., M. Hoferichter, T. Bhattacharya, E. Mereghetti, B. Yoon and S. Park. The pion-nucleon sigma term from Lattice QCD. Presented at *The 10th International*

Workshop on Chiral Dynamics. (Beijing, China, 2021-11-15 - 2021-11-19). (LA-UR-22-22580)

Gupta, R., M. Hoferichter, T. Bhattacharya, V. Cirigliano, E. Mereghetti, Y. C. Jang, B. Joo, F. Winter, B. Yoon, S. Park and S. Mondal. Excited states and precision results for nucleon charges and form factor. Presented at *The 38th International Symposium on Lattice Field Theory, LATTICE2021 26th-30th July, 2021 Zoom/ Gather@Massachusetts Institute of Technology*. (Cambridge, Massachusetts, United States, 2021-07-26 - 2021-07-30). (LA-UR-21-32449)

Mondal, S., T. Bhattacharya, R. Gupta, B. Jo\xc3\xb3, H. Lin, S. Park, F. Winter and B. Yoon. Nucleon isovector momentum fraction, helicity and transversity moment using Lattice QCD. Presented at *The 38th International Symposium on Lattice Field Theory*. (Boston, Massachusetts, United States, 2021-07-26 - 2021-07-30). (LA-UR-21-32143)

Zhang, R., T. Bhattacharya, R. Gupta, H. W. Lin, S. Mondal, S. Park and B. Yoon. Strange and charm contributions to nucleon charges and moments. Presented at *The 38th International Symposium on Lattice Field Theory, LATTICE2021*. (Boston, Massachusetts, United States, 2021-07-26 - 2021-07-30). (LA-UR-21-28804)

Books/Chapters

Gupta, R., T. Bhattacharya and B. Yoon. ML and Theoretical Particle Physics. (LA-UR-22-22125)

Presentation Slides

Bhattacharya, T. Calculating neutron properties to look for new physics. . (LA-UR-21-22554)

Clayton, S. Testing the Standard Model of Particle Physics with Neutron Decay. Presented at *Los Alamos National Laboratory P/T Colloquium*, Los Alamos, New Mexico, United States, 2021-08-26 - 2021-08-26. (LA-UR-21-28482)

Clayton, S. Precision measurements of neutron beta decay - CERN EP seminar. Presented at *CERN EP seminar - Virtual*, Geneva, Switzerland, 2022-01-25 - 2022-01-25. (LA-UR-22-20542)

Gupta, R. Unitarity of CKM Matrix: |Vud| from neutron decay. Presented at *Snowmass RF02 Topical group*, Virtual, New Mexico, United States, 2020-10-02 - 2020-10-02. (LA-UR-21-20528)

Gupta, R. Lattice QCD at LANL (2020 PR). . (LA-UR-21-22424)

Gupta, R. Overview of HEP Theory and QuantISED Efforts and Nucleon Matrix elements. Presented at *DOE HEP Review*, Virtual, New Mexico, United States, 2021-07-06 - 2021-07-08. (LA-CP-21-20598)

Gupta, R. Excited states and precision results for nucleon charges and form factors. Presented at *38 International Symposium on Lattice Field Theory, 2021*, Boston (virtual), Massachusetts, United States, 2021-07-26 - 2021-07-26. (LA-UR-21-27234)

Gupta, R. Simulations of Lattice QCD Come of Age. Presented at *Rajan Gupta*, Los ALamos, New Mexico, United States, 2021-12-09 - 2021-12-09. (LA-UR-21-32028)

Gupta, R., H. Lin, B. Yoon, S. Mondal, T. Bhattacharya and S. Park. Flavor diagonal matrix elements. Presented at *USQCD all hands meeting*, Boston (virtual), Massachusetts, United States, 2021-04-30 - 2021-04-30. (LA-UR-21-24214)

Gupta, R., M. Hoferichter, E. Mereghetti, T. Bhattacharya, B. Yoon and S. Park. The pion–nucleon sigma term from lattice QCD. Presented at *Chiral Dynamics 2021*, Beijing, China, 2021-11-15 - 2021-11-15. (LA-UR-21-31181)

Gupta, R., T. Bhattacharya, E. Mereghetti, B. Yoon, S. Mondal and S. Park. Radiative corrections to Vud: Calculation of the \xce\xb3 – W box diagram using Lattice QCD. . (LA-UR-21-22629)

Mereghetti, E. beta decays to probe physics beyond the Standard Model. . (LA-UR-22-22585)

Wang, Z. Ultracold Neutron (UCN) quantum states & Position-sensitive measurements. Presented at *LANL UCN Beta Decay Collaboration Meeting*, Los Alamos, New Mexico, United States, 2020-11-24 - 2020-11-24. (LA-UR-20-29798)

Wang, Z. Detecting neutrons, from ultra-hot to ultra-cold energies. . (LA-UR-21-25232)

High-fidelity Electromagnetic Simulation Capability for Inertial Confinement Fusion (ICF)/High Energy Density (HED) Experiments

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Project Description

This project intends to develop and demonstrate a high-fidelity simulation capability for High Energy Density (HED) and Inertial Confinement Fusion (ICF) experiments. The proposed work is critically important for the United States national security and the Los Alamos National Laboratory mission. Achieving ICF ignition in the laboratory remains critical for the stockpile stewardship program. This project will have a direct mission impact not only by assessing paths towards ignition, but also by enabling new understanding of HED experiments that use hohlraums and similar environments. Our simulation tool will also help us comprehend essential physics missing from current weapons simulation codes and assess how to incorporate them.

Publications

Journal Articles

Anderson, S. E., L. Chacon, W. Taitano, A. N. Simakov and B. Keenan. Fully kinetic simulations of strong steady-state collisional planar plasma shocks. 2021. *Physical Review E*. **104** (5): 055205. (LA-UR-21-25938 DOI: 10.1103/PhysRevE.104.055205)

Simakov, A. N. Electron transport in a collisional plasma with multiple ion species in the presence of a magnetic field. Submitted to *Physics of Plasmas*. (LA-UR-21-30844)

Conference Papers

Hammer, H. R., H. Park, L. Chacon, W. Taitano, S. E. Anderson and A. N. Simakov. A coupled radiation-diffusion and kinetic plasma physics solver. Presented at *The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021)*. (Raleigh, North Carolina, United States, 2021-10-03 - 2021-10-07). (LA-UR-21-21579)

Presentation Slides

Anderson, S. E. Hohlraum Kinetic Plasma Interpenetration and Mix. . (LA-UR-22-21597)

Anderson, S. E., L. Chacon, A. N. Simakov, B. Keenan and W. Taitano. Overview of iFP kinetic electrons capability. Presented at *MIT kinetic experiments meeting*, Online, New Mexico, United States, 2021-09-29 - 2021-09-29. (LA-UR-21-29667)

Anderson, S. E., L. Chacon, W. Taitano, A. N. Simakov and B. Keenan. Fully kinetic simulations of collisional plasma shocks. Presented at *63rd Annual meeting of APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30792)

Chacon, L. Modern implicit algorithms for multiscale kinetic plasma simulation. Presented at *2nd Computational Physics School for Fusion Research*, Virtual, Massachusetts, United States, 2021-08-30 - 2021-08-30. (LA-UR-21-28346)

Chacon, L., G. Chen, A. J. Stanier and B. Philip. Report Viewgraphs for IC Project "High-fidelity Electromagnetic Simulation Capability for ICF/HED Experiments" (w21_ampgpu). . (LA-UR-22-21682)

Chacon, L. and B. M. Haines. Computational Physics Challenges in ICF/HED (part II). . (LA-UR-22-22103)

Hammer, H. R., H. Park, L. Chacon, W. Taitano, S. E. Anderson and A. N. Simakov. Coupled radiation transport and plasma physics for ICF simulations. . (LA-UR-21-29053)

Hammer, H. R., H. Park, L. Chacon, W. Taitano, S. E. Anderson and A. N. Simakov. A coupled radiation-diffusion and kinetic plasma physics solver for ICF simulations. Presented at *ANS M&C 2021 - The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Raleigh, North Carolina, United States, 2021-10-03 - 2021-10-07. (LA-UR-21-29443)

Yin, L. IC Report for project "Developing nonlinear laser-plasma instability models for high-fidelity, multi-physics simulation capability for ICF/HED". . (LA-UR-22-21536)

Yin, L., T. B. Nguyen, G. Chen, L. Chacon, D. J. Stark, L. M. Green and B. M. Haines. Nonlinear physics of cross-beam energy transfer relevant to indirect drive ignition inertial confinement fusion experiments. Presented at *63rd Annual Meeting of the American Physical Society Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30746)

Adaptive Machine Learning for Closely Spaced Ultra-Short Intense Accelerator Beams

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Project Description

Particle accelerators are some of the most useful tools for research because of their ability to probe the interior of subatomic particles, to provide extremely bright and short flashes of X-rays that capture the dynamics of shockwaves, chemical, and biological processes, to produce images of explosion-driven shock wave dynamics in large samples, and for medical isotope production. Accelerators are extremely powerful, large, complex machines with thousands of interconnected components that drift with time and beams that must be tightly focused and precisely accelerated while undergoing complicated nonlinear motion. The main goals of this project are to develop physics-informed adaptive machine learning tools to create controls and diagnostics that improve the performance of all existing accelerators and enable the creation of new machines with beyond state-of-the-art capabilities. In particular, our tools are meant to: 1) decrease the large amounts of wasted time and money in re-tuning after a shut down or to make large parameter changes between various experiments, 2) optimize the current suboptimal performance of operating accelerators by automatically adjusting as beams and accelerator components drift with time, 3) overcome fundamental limitations such as an inability to accelerate trains of closely spaced high intensity charged particle bunches in efficient structures.

Publications

Journal Articles

Diaw, A., M. McKerns, I. Sagert, L. G. Stanton and M. S. Murillo. Efficient Learning of Accurate Surrogates for Simulations of Complex Systems. Submitted to *Nature Machine Intelligence*. (LA-UR-20-24947)

Pavlenko, V., J. M. Smedley, A. Scheinker, R. L. Fleming, A. M. Alexander, M. A. Hoffbauer and N. A. Moody. Stoichiometry control and automated growth of alkali antimonide photocathode films by molecular beam deposition. Submitted to *Applied Physics Letters*. (LA-UR-21-30432)

*Scheinker, A. Adaptive Machine Learning for Robust Diagnostics and Control of Time-Varying Particle Accelerator Components and Beams. 2021. *Information*. **12** (4): 161. (LA-UR-21-24256 DOI: 10.3390/info12040161)

Scheinker, A. Adaptive Machine Learning for Time-Varying Systems: Low Dimensional Latent Space Tuning. Submitted to *Journal of Instrumentation*. (LA-UR-21-26483)

Scheinker, A., E. Huang and C. E. Taylor. Extremum Seeking-Based Control System for Particle Accelerator Beam Loss Minimization. 2021. *IEEE Transactions on Control Systems Technology*. (LA-UR-21-24323 DOI: 10.1109/TCST.2021.3136133)

Conference Papers

Scheinker, A. Adaptive Machine Learning for Time-Varying Particle Accelerators and Beams. Presented at *AI@DOE*. (Los Alamos, New Mexico, United States, 2022-02-28 - 2022-02-28). (LA-UR-22-21859)

Reports

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Unpublished report. (LA-UR-21-24972)

Presentation Slides

McKerns, M. mystic: physics-informed learning and automated design/control under uncertainty. Presented at *Applied Machine Learning Symposium*, Los Alamos, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-27369)

McKerns, M. mystic: software for autonomous discovery and design under uncertainty. Presented at *CAMERA Workshop on Autonomous Discovery in Science and Engineering*, Berkeley, California, United States, 2021-04-20 - 2021-04-22. (LA-UR-21-30257)

Pavlenko, V. Automated growth of photocathode films: from the basics of process control towards artificial intelligence. Presented at *Photocathode Physics for Photoinjectors (P3) Workshop*, Menlo Park, California, United States, 2021-11-10 - 2021-11-12. (LA-UR-21-31176)

Pavlenko, V. Automated Growth of Photocathodes. . (LA-UR-22-20586)

Scheinker, A. Adaptive Feedback and Machine Learning for Time-Varying Particle Accelerator Systems. Presented at *FRIB accelerator physics and engineering seminars*, East Lansing, Michigan, United States, 2021-02-19 - 2021-02-19. (LA-UR-21-21382)

Scheinker, A. Adaptive Machine Learning for Time-Varying Systems. Presented at *OWLE seminar at PSI*, Los Alamos, New Mexico, United States, 2021-05-27 - 2021-05-27. (LA-UR-21-24255)

Scheinker, A. Adaptive Machine Learning and Feedback Controls for Particle Accelerators. Presented at *EPICS meeting*, Los Alamos, New Mexico, United States, 2021-07-21 - 2021-07-23. (LA-UR-21-26509)

Scheinker, A. Adaptive Control and Machine Learning for Particle Accelerator Beam Control and Diagnostics. Presented at *10th International Beam Instrumentation Conference*, Seoul, Korea, South, 2021-09-13 - 2021-09-13. (LA-UR-21-28896)

Scheinker, A. Adaptive Machine Learning for Control and Virtual Diagnostics of Time-Varying Particle Accelerator Systems and Beams. Presented at *AI for Particle Accelerators, X-ray Beamlines, and Electron Microscopy Workshop @ ANL*, Lemont, Illinois, United States, 2021-11-01 - 2021-11-01. (LA-UR-21-30943)

Scheinker, A. Adaptive Machine Learning for Automatic Control and Non-invasive Diagnostics of Time- Varying Charged Particle Beams. Presented at *ML for accelerators meeting*, Los Alamos, New Mexico, United States, 2021-12-01 - 2021-12-01. (LA-UR-21-31583)

Scheinker, A. Adaptive Machine Learning for Particle Accelerator Tuning. Presented at *Extreme Storage Rings Workshop 2022*, Los Alamos, New Mexico, United States, 2022-01-31 - 2022-01-31. (LA-UR-22-20999)

A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility

Mark Schmitt
20180051DR

Project Description

We will investigate key aspects of achieving ignition using direct laser drive of a triple shell implosion system. The achievement of fusion in the laboratory is a grand challenge problem whose solution would be recognized worldwide and advance research in both fusion energy and weapons science. If successful, a completely new venue for experiments to understand and explore the conditions of ignition in the laboratory would be born.

Technical Outcomes

Experiments on Omega and the National Ignition Facility (NIF) validated the basic physics assumptions of the Revolver ignition concept including high laser coupling to the target (>90%) and as-predicted kinetic collision efficiency between shells. Theoretical analysis confirmed the stability of the Revolver triple shell design and its lack of significant diffusive mix into the fuel. Fabrication of multi-shell capsules incorporating low-density inter-shell 3D-printed lattice materials was demonstrated and used in experiments to measure asymmetry perturbations up to mode 40.

Publications

Journal Articles

*Keenan, B. D., W. T. Taitano and K. Molvig. Physics of the implosion up until the time of ignition in a revolver (triple-shell) capsule. 2020. *Physics of Plasmas*. **27** (4): 042704. (LA-UR-20-20116 DOI: 10.1063/1.5143888)

*Krasheninnikova, N. S., M. J. Schmitt, K. Molvig, S. C. Hsu, B. S. Scheiner, D. W. Schmidt, V. Geppert-Kleinrath, P. W. McKenty, D. T. Michel, D. H. Edgell, F. J. Marshall and H. Huang. Development of a directly driven multi-shell platform: Laser drive energetics. 2020. *Physics of Plasmas*. **27** (2): 22706. (LA-UR-19-23347 DOI: 10.1063/1.5100518)

*Molvig, K., M. J. Schmitt, R. Betti, E. M. Campbell and P. McKenty. Stable and confined burn in a Revolver ignition capsule. 2018. *Physics of Plasmas*. **25** (8): 82708. (LA-UR-18-23353 DOI: 10.1063/1.5037224)

Scheiner, B. S., M. J. Schmitt, D. W. Schmidt, L. A. Goodwin, F. J. Marshall and P. Nilson. Two-photon polymerization printed lattices as support structures in multi-shell ICF targets: Platform development and initial assessment. Submitted to *Physics of Plasmas*. (LA-UR-20-26243)

Scheiner, B. S. and M. J. Schmitt. The role of incidence angle in the laser ablation of ICF targets. Submitted to *Physics of Plasmas*. (LA-UR-18-24731)

Scheiner, B. S. and M. J. Schmitt. Considerations for the modeling of the laser ablation region of ICF targets with Lagrangian simulations. 2021. *AIP Advances*. **11** (10): 105208. (LA-UR-20-20032 DOI: 10.1063/5.0056006)

*Scheiner, B., M. J. Schmitt, S. C. Hsu, D. Schmidt, J. Mance, C. Wilde, D. N. Polsin, T. R. Boehly, F. J. Marshall, N. Krasheninnikova, K. Molvig and H. Huang. First experiments on Revolver shell collisions at the OMEGA laser. 2019. *Physics of Plasmas*. **26** (7): 072707. (LA-UR-19-23222 DOI: 10.1063/1.5099975)

*Scheiner, B. and M. Schmitt. The role of incidence angle in the laser ablation of a planar target. 2019. *Physics of Plasmas*. **26** (2): 24502. (LA-UR-18-29321 DOI: 10.1063/1.5085122)

Taitano, W., B. Keenan, L. Chacon, A. N. Simakov, S. E. Anderson, H. R. Hammer and B. J. Albright. An Eulerian Vlasov-Fokker-Planck Algorithm for Spherical Implosion Simulations of Inertial Confinement Fusion Capsules. Submitted to *Computer Physics Communications*. (LA-UR-20-26872)

Presentation Slides

Keenan, B., W. Taitano and K. Molvig. Revolver Implosion Physics Up Until the Time of Ignition. Presented at *American Physical Society Division of Plasma Physics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28911)

Kyrala, G. A., T. J. Murphy, N. S. Vinyard and M. J. Schmitt. Comparing Backlighter Images at NIF to calculations. Presented at *Anomalous Absorption ZCOnference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-09. (LA-UR-19-25366)

Molvig, K., M. J. Schmitt, R. Betti, E. M. Campbell and P. McKenty. The Revolver Ignition Capsule: Persistent stagnation and high efficiency burn. . (LA-UR-17-31342)

Molvig, K. and M. J. Schmitt. Pointing scheme for the NIF laser with "perfect" low mode uniformity. Presented at *The 61st Annual Meeting of the APS Division of Plasma Physics*, Ft. Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30763)

Scheiner, B. S. Revolver 19A Omega Results. . (LA-UR-19-21123)

Scheiner, B. S., M. J. Schmitt, D. W. Schmidt, F. J. Marshall and P. M. Nilson. Revolver-20B Prewatch Brief. . (LA-UR-20-27419)

Scheiner, B. S., M. J. Schmitt, D. W. Schmidt, F. J. Marshall and P. Nilson. Monday Experimental Meeting Results: Revolver 20C. Presented at *Weekly Experimental Meeting at the Laboratory for Laser Energetics*, Rochester, New York, United States, 2020-11-16 - 2020-11-16. (LA-UR-20-29348)

Scheiner, B. S., M. J. Schmitt, D. W. Schmidt, F. Marshall, C. H. Wilde and P. Adrian. Revolver-20A Campaign Preview. . (LA-UR-19-32065)

Scheiner, B. S., M. J. Schmitt, D. W. Schmidt, L. A. Goodwin and F. J. Marshall. Exploration of the use of two-photon polymerization printed structures in multi-shell ICF targets. Presented at *APS Division of Plasma Physics Meeting*, Online, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28893)

Scheiner, B. S., M. J. Schmitt, J. Mance, D. W. Schmidt, D. N. Polsin, F. J. Marshall, P. Nilson and C. H. Wilde. Revolver-19B Campaign Preview. . (LA-UR-19-28625)

Schmidt, D. W., T. Cardenas, T. H. Day, P. M. Donovan, F. Fierro, L. A. Goodwin, M. J. Herman, J. C. Lamar, L. A. Kuettner, B. M. Patterson, T. E. Quintana, R. B. Randolph, B. S. Scheiner, M. J. Schmitt, O. C. Trautschold, D. R. Vodnik, C. T. Wilson, H. Huang, C. Shuldberg and T. Drake. Target Fabrication Efforts for Multi-Shell Direct Drive. Presented at *Target Fabrication Speacilists*, Anapolis, Massachusetts, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23462)

Schmitt, M. J., B. S. Scheiner, D. W. Schmidt, L. Kot, M. J. Rosenberg, C. H. Wilde, H. Huang, P. W. McKenty, B. Keenan and K. Molvig. First directly-driven double shell implosions on the National Ignition Facility. Presented at *Annual American Physical Society Division of Plasma Physics*, Memphis, Tennessee, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29178)

Schmitt, M. J., K. Molvig, B. S. Scheiner, C. H. Wilde, N. S. Vinyard, D. W. Schmidt, S. C. Hsu, T. A. Gianakon, L. Kot, M. J. Rosenberg, F. J. Marshall, D. Edgell, P. W. McKenty, D. N. Polsin, R. S. Craxton and H. Huang. Progress in advancing the Revolver triple-shell direct-drive ignition concept. Presented at *American Physical Society Division of Plasma Physics Conference*, Ft Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30727)

Schmitt, M. J., K. Molvig, B. S. Scheiner, C. H. Wilde, N. S. Vinyard, D. W. Schmidt, S. C. Hsu, T. A. Gianakon, L. Kot, M.

J. Rosenberg, F. J. Marshall, D. Edgell, P. W. McKenty, D. N. Polsin, R. S. Craxton, H. Huang and J. G. Mance. Progress in advancing the Revolver triple-shell direct-drive ignition concept. . (LA-UR-19-31695)

Schmitt, M. J., K. Molvig, B. S. Scheiner, N. S. Vinyard, C. H. Wilde, D. W. Schmidt, L. Kot, S. C. Hsu, P. W. (. McKenty, M. Rosenberg, D. Turnbull, M. Hohenberger and H. Huang. Rad-hydro simulations of the Revolver direct-drive multi-shell ignition concept. Presented at *International Conference on High Energy Density (ICHED) 2019*, Oxford, United Kingdom, 2019-04-01 - 2019-04-05. (LA-UR-19-22857)

Schmitt, M. J., K. Molvig, B. S. Scheiner, N. S. Vinyard, P. McKenty, D. Edgell, T. Michel and F. Marshall. 2-Dimensional simulations of the Revolver direct-drive multi-shell ignition concept. Presented at *48th Annual Anomalous Absorption Conference*, Bar Harbor, Maine, United States, 2018-07-09 - 2018-07-13. (LA-UR-18-26304)

Schmitt, M. J., K. Molvig, B. S. Scheiner, N. S. Vinyard, S. C. Hsu, T. A. Gianakon and D. W. Schmidt. A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility. . (LA-UR-18-31102)

Schmitt, M. J., K. Molvig, D. W. Schmidt, B. S. Scheiner, C. H. Wilde, T. A. Gianakon, B. Keenan and A. N. Black. LDRD-DR Project Appraisal: A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility. . (LA-UR-20-21789)

Schmitt, M. J., K. Molvig, N. S. Vinyard, B. S. Scheiner, D. W. Schmidt, S. C. Hsu, C. H. Wilde, L. Kot, D. Edgell, F. Marshall, P. McKenty, M. Rosenberg, D. Turnbull, M. Hohenberger and H. Huang. Physics-driven target requirements for the Revolver direct-drive triple-shell ignition concept. Presented at *Target Fabrication Workshop*, Annapolis, Maryland, United States, 2019-04-22 - 2019-04-26. (LA-UR-19-23624)

Schmitt, M. J., N. S. Vinyard, B. S. Scheiner, K. Molvig, A. Zylstra, C. H. Wilde, D. W. Schmidt, P. McKenty, M. Rosenberg, D. Turnbull, J. Di Nicola, G. Guruangan, M. Hohenberger, P. Di Nicola, B. MacGowan, T. Zobrist, H. Huang and M. Schoff. Multi-Shell Direct-Drive Ablator Energetics Campaign: P-000428. Presented at *HED/ICF Council & PRP Meeting*, Livermore, California, United States, 2018-08-28 - 2018-08-30. (LA-UR-18-27730)

Schmitt, M. J., N. S. Vinyard, B. S. Scheiner, K. Molvig, C. H. Wilde, D. W. Schmidt, P. W. McKenty, M. Rosenberg, D. Turnbull, M. Hohenberger, H. Huang and L. Kot. Direct-Drive Multi-Shell (DDMS) Collision Energetics: ABLE P-000515. Presented at *ICF Council Meeting for NIF shots*, Livermore, California, United States, 2019-03-05 - 2019-03-05. (LA-UR-19-21451)

Schmitt, M. J., R. E. Olson, B. S. Scheiner and B. M. Haines. The Quest for Inertial Confinement Fusion using Large Directly Driven Targets with 1, 2 or 3 Concentric Shells. . (LA-UR-21-31880)

Schmitt, M. J. and C. H. Wilde. Multi-Shell Direct-Drive Ablator Energetics (ABLE). . (LA-UR-20-21770)

Posters

I. Magrogan, W. R., B. S. Scheiner and M. J. Schmitt. Performance impacts of Beam Width on Direct Drive ICF. Presented at *60th Annual Meeting of the APS Division of Plasma Physics Co-Located with the 71st Annual Gaseous Electronics Conference*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30401)

Scheiner, B. S. and M. J. Schmitt. Understanding the role of incidence angle in PDD. Presented at *Omega Laser Users Group Workshop*, Rochester, New York, United States, 2018-04-25 - 2018-04-25. (LA-UR-18-23461)

Scheiner, B. S. and M. J. Schmitt. The Role of Incidence Angle in the Laser Ablation of ICF Targets. Presented at *Anomalous Absorption Conference*, Bar Harbor, Maine, United States, 2018-07-08 - 2018-07-08. (LA-UR-18-26080)

Scheiner, B. S. and M. J. Schmitt. The Role of Incidence Angle in the Laser Ablation of ICF Targets. Presented at *APS DPP meeting*, Portland, Oregon, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30399)

Schmitt, M. J., K. Molvig, N. S. Vinyard, S. C. Hsu, B. S. Scheiner, V. Geppert-Kleinrath, D. W. Schmidt, P. McKenty, T. Michel, D. Edgell, F. Marshall, R. Betti, M. Campbell and H. Huang. The Revolver direct-drive Ignition concept: Ignition platform and burning plasma testbed. Presented at *Weapons science capability review*, Los Alamos, New Mexico, United States, 2018-04-16 - 2018-04-16. (LA-UR-18-23059)

Nucleosynthesis Probes of Cosmic Explosions

Christopher Fryer
20190021DR

Project Description

Multi-physics modeling, combining transport, nuclear physics, and hydrodynamics all play an important role in a range of problems of national interest. This project brings together both physics experts and computational scientists to study the multi-physics problem surrounding the emission of from the merger of two neutron stars. The physics components and the numerical methods used to combine these physics components will develop techniques Los Alamos scientists will be able to use throughout the Advanced Simulation and Computing (ASC) program.

Technical Outcomes

This project developed a holistic approach to studying the uncertainties in calculating neutron star merger light-curves and hence, uncertainties in our ability to infer r-process masses from observations of these mergers. This approach required the inclusion of a broad set of microphysics into multiple large-scale codes, tightly coupled together. The project placed Los Alamos as a world leader in these calculations, leading to a broad range of national and international collaboration.

Publications

Journal Articles

Al-Mamun, M., A. W. Steiner, J. Nattila, J. Lange, R. O'Shaughnessy, I. Tews, S. Gandolfi, C. Heinke and S. Han. Combining Electromagnetic and Gravitational-Wave Constraints on Neutron-Star Masses and Radii. Submitted to *Physical Review Letters*. (LA-UR-20-26423)

*Banerjee, S., K. Belczynski, C. L. Fryer, P. Berczik, J. R. Hurley, R. Spurzem and L. Wang. BSE versus StarTrack: Implementations of new wind, remnant-formation, and natal-kick schemes in NBODY7 and their astrophysical consequences. 2020. *Astronomy & Astrophysics*. **639**. (LA-UR-20-22131 DOI: 10.1051/0004-6361/201935332)

Barnes, J., Y. L. Zhu, K. A. Lund, T. M. Sprouse, N. Vassh, G. C. McLaughlin, M. R. Mumpower and R. Surman. Kilonovae across the nuclear physics landscape: the impact of nuclear physics uncertainties on r-process-powered emission. Submitted to *Astrophysical Journal*. (LA-UR-20-28560)

Belczynski, K., T. Bulik, A. Olejak, M. Chru\xc5\x9bli\xc5\x84ska, N. Singh, N. Pol, L. Zdunik, R. O'Shaughnessy, M. McLaughlin, D. Lorimer, O. Korobkin, E. van den Heuvel, M. B. Davies and D. E. Holz. Binary neutron star formation and the origin of GW170817. Submitted to *Astronomy and Astrophysics*. (LA-UR-19-20692)

Braun, C., S. Safi-Harb and C. L. Fryer. Chandra and XMM–Newton Study of the Supernova Remnant RCW 103 (G332.4–0.4) Containing the Peculiar Central Compact Object 1E 161348–5055. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-18-31702)

*Braun, C., S. Safi-Harb and C. L. Fryer. Progenitors and explosion properties of supernova remnants hosting central compact objects: I. RCW \xe2\x80\x89103 associated with the peculiar source 1E \xe2\x80\x89161348–5055. 2019. *Monthly Notices of the Royal Astronomical Society*. **489** (3): 4444-4463. (LA-UR-19-24543 DOI: 10.1093/mnras/stz2437)

*Burrows, A., D. Radice, D. Vartanyan, H. Nagakura, M. A. Skinner and J. C. Dolence. The overarching framework of core-collapse supernova explosions as revealed by 3D fornax simulations. 2020. *Monthly Notices of the Royal Astronomical Society*. **491** (2): 2715-2735. (LA-UR-19-28512 DOI: 10.1093/mnras/stz3223)

C\xc3\xb4t\xc3\xa9, B., P. Denissenkov, F. Herwig, C. L. Fryer, K. Belczynski, N. Vassh, M. R. Mumpower, J. Lippuner, M. Pignatari and A. J. Ruiter. The Impact of Nuclear Physics Uncertainties on Galactic Chemical Evolution Predictions. 2020. *Journal of Physics: Conference Series*. **1668** (1): 12008. (LA-UR-20-20369 DOI: 10.1088/1742-6596/1668/1/012008)

Cakirli, R. B., R. F. Casten and A. J. Couture. Effects of shape/phase transition regions on r-process neutron capture cross sections. Submitted to *Physical Review C*. (LA-UR-21-28318)

Chase, E. A., B. O'Connor, C. L. Fryer, E. Troja, O. Korobkin, R. T. Wollaeger, E. Holmbeck, M. Ristic, C. J. Fontes, A. L. Hungerford and A. M. Herring. Kilonova Detectability with Wide-Field Instruments. Submitted to *Astrophysical Journal*. (LA-UR-21-24587)

*Chatzopoulos, E., M. S. Gilmer, R. T. Wollaeger, C. Frohlich and W. P. Even. Synthetic Spectra of Pair-instability Supernovae in 3D. 2019. *The Astrophysical Journal*. **875** (2): 140. (LA-UR-19-21458 DOI: 10.3847/1538-4357/ab1082)

Cote, B., M. Eichler, A. Yague, N. Vassh, M. R. Mumpower, B. Vilagos, B. Soos, A. Arcones, T. M. Sprouse, R. Surman, M. Pignatari, B. Wehmeyer, T. Rauscher and M. Lugaro. Constraining the rapid neutron-capture process with meteoritic 129-I and 247-Cm. Submitted to *Science*. (LA-UR-19-30942)

Couture, A. J., R. Casten and R. B. Cakirli. Improved Predictions for r-process Cross Sections. Submitted to *Nuclear Physics News International*. (LA-UR-19-25512)

Couture, A. J., R. F. Casten and R. B. Cakirli. Significantly improved estimates of neutron capture cross sections relevant to the r process. Submitted to *Physical Review C*. (LA-UR-21-28653)

Curtis, S., N. M. Lloyd Ronning, J. M. Miller and C. Frohlich. Full Transport GRRMHD for Kilonovae from Black Hole—Neutron Star Merger Disks. Submitted to *Astrophysical Journal*. (LA-UR-20-27560)

Dichiara, S., R. L. Becerra, E. Troja, E. A. Chase, W. H. Lee, A. M. Watson, N. R. Butler, B. O'Connor, M. Pereyra, K. O. C. Lopez, A. Y. Lien, A. Gottlieb and A. S. Kutyrev. CONSTRAINTS ON THE ELECTROMAGNETIC COUNTERPART OF THE NEUTRON STAR BLACK HOLE MERGER GW200115. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-30129)

*Doctor, Z., R. Kessler, K. Herner, A. Palmese, M. Soares-Santos, J. Annis, D. Brout, D. E. Holz, M. Sako, A. Rest, P. Cowperthwaite, E. Berger, R. J. Foley, C. J. Conselice, M. S. S. Gill, S. Allam, E. Balbinot, R. E. Butler, H. -. Chen, R. Chornock, E. Cook, H. T. Diehl, B. Farr, W. Fong, J. Frieman, C. Fryer, J. Garcia-Bellido, R. Margutti, J. L. Marshall, T. Matheson, B. D. Metzger, M. Nicholl, F. Paz-Chinchon, S. Salim, M. Sauseda, L. F. Secco, R. C. Smith, N. Smith, A. K. Vivas, D. L. Tucker, T. M. C. Abbott, S. Avila, K. Bechtol, E. Bertin, D. Brooks, E. Buckley-Geer, D. L. Burke, A. Carnero Rosell, M. C. Kind, J. Carretero, F. J. Castander, C. B. D'Andrea, L. N. da Costa, J. De Vicente, S. Desai, P. Doel, B. Flaugher, P. Fosalba, E. Gaztanaga, D. W. Gerdes, D. A. Goldstein, D. Gruen, R. A. Gruendl, G. Gutierrez, W. G. Hartley, D. L. Hollowood, K. Honscheid, B. Hoyle, D. J. James, T. Jeltema, S. Kent, K. Kuehn, N. Kuropatkin, O. Lahav, M. Lima, M. A. G. Maia, M. March, F. Menanteau, C. J. Miller, R. Miquel, E. Neilsen, B. Nord, R. L. C. Ogando, A. A. Plazas, A. Roodman, E. Sanchez, V. Scarpine, R. Schindler, M. Schubnell, S. Serrano, I. Sevilla-Noarbe, M. Smith, F. Sobreira, E. Suchyta, M. E. C. Swanson, G. Tarle, D. Thomas, A. R. Walker and W. Wester. A Search for Optical Emission from Binary Black Hole Merger GW170814 with the Dark Energy Camera. 2019. *The Astrophysical Journal Letters*. **873** (2): L24. (LA-UR-18-31578 DOI: 10.3847/2041-8213/ab08a3)

Drozda, P., K. Belczynski, R. O'Shaugnessy, T. Bulik and C. L. Fryer. Black hole–neutron star mergers: the first mass gap and kilonovae. Submitted to *Astronomy and Astrophysics*. (LA-UR-20-27532)

Eichler, M., W. Sayar, A. Arcones and O. Korobkin. WHAT IS THE ORIGIN OF ACTINIDE-BOOST STARS?. Submitted to *Astrophysical Journal*. (LA-UR-18-31556)

Even, W. P., O. Korobkin, C. L. Fryer, C. J. Fontes, R. T. Wollaeger, A. L. Hungerford, J. Lippuner, J. M. Miller, M. R. Mumpower and G. W. Misch. Composition Effects on Kilonova Spectra and Light Curves: I. Submitted to *Astrophysical Journal*. (LA-UR-19-23935)

Fong, W. F., T. Laskar, J. Rastinejad, A. Rouco Escorial, G. Schroeder, C. D. Kilpatrick, K. Paterson, J. Barnes, E. Berger, B. D. Metzger, Y. Dong, A. Nugent, R. Strausbaugh, P. Blanchard, A. Goyal, A. Cucchiara, G. Terreran, K. D. Alexander, T. Eftekhari, C. L. Fryer, B. Margalit, R. Margutti and M. Nicholl. The Broad-band Counterpart of the Short GRB 200522A at z = 0:5536: A Luminous Kilonova or a Collimated Outflow with a Reverse Shock?. Submitted to *Astrophysical Journal*. (LA-UR-20-26506)

*Fontes, C. J., C. L. Fryer, A. L. Hungerford, R. T. Wollaeger and O. Korobkin. A line-binned treatment of opacities for the spectra and light curves from neutron star mergers. 2020. *Monthly Notices of the Royal Astronomical Society*. **493** (3): 4143-4171. (LA-UR-19-21612 DOI: 10.1093/mnras/staa485)

Fontes, C. J., C. L. Fryer, R. T. Wollaeger, M. R. Mumpower and T. M. Sprouse. Actinide opacities for modeling the spectra and light curves from neutron star mergers. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-31109)

Fryer, C. L., C. J. Fontes, J. S. Warsa, P. W. Roming, S. X. Coffing and S. Wood. The role of Inhomogeneities in Supernova Shock Breakout Emission. Submitted to *Astrophysical Journal*. (LA-UR-19-32532)

*Fryer, C. L., N. Lloyd-Ronning, R. Wollaeger, B. Wiggins, J. Miller, J. Dolence, B. Ryan and C. E. Fields. Understanding the engines and progenitors of gamma-ray bursts. 2019. *European Journal of Physics*. **55** (8): 132. (LA-UR-19-20858 DOI: 10.1140/epja/i2019-12818-y)

Fryer, C. L., P. Karpov and D. Livescu. Understanding Convection in the Core-Collapse Supernova Engine. Submitted to *Astronomy Reports*. (LA-UR-20-29683)

Graesser, M. L., I. Shoemaker and N. Tapia Arellano. Milli-Magnetic Dark Matter and the Survival of Galactic Magnetic Fields. Submitted to *High Energy Density Physics*. (LA-UR-21-20891)

Graesser, M. L., I. Shoemaker and N. Tapia Arellano. Milli-Magnetic Monopole Dark Matter and the Survival of Galactic Magnetic Fields. Submitted to *Journal of High Energy Physics*. (LA-UR-21-24525)

Holmbeck, E., A. Frebel, G. C. McLaughlin, R. Surman, R. Fernandez, B. D. Metzger, M. R. Mumpower and T. M.

Sprouse. Reconstructing masses of merging neutron stars from stellar r-process abundance signatures. Submitted to *Astrophysical Journal*. (LA-UR-20-27862)

Huth, S., P. T. Pang, I. Tews, A. Le Fevre, T. Dietrich, M. W. Coughlin and A. Schwenk. Constraining Dense Nuclear Matter with Microscopic and Macroscopic Collisions. Submitted to *Physical Review Letters*. (LA-UR-21-22072)

Janiuk, A. and O. Korobkin. The imprint of r-process nucleosynthesis in the outflows from GRB accretion disks on their observable properties. Submitted to *Astrophysical Journal*. (LA-UR-18-31470)

*W. R. T. *. F. C. L. *. H. A. L. *. R. S. *. F. C. J. *. M. M. R. *. C. E. A. *. E. W. P. *. M. J. *. M. G. W. *. L. J. Korobkin, O. *., O. Korobkin, R. T. Wollaeger, C. L. Fryer, A. L. Hungerford, C. J. Fontes, M. R. Mumpower, E. A. Chase, W. P. Even, G. W. Misch, J. Lippuner and J. Miller. Axisymmetric Radiative Transfer Models of Kilonovae. 2021. *The Astrophysical Journal*. **910** (2): 116. (LA-UR-20-22607 DOI: 10.3847/1538-4357/abe1b5)

*Korobkin, O., A. M. Hungerford, C. L. Fryer, M. R. Mumpower, G. W. Misch, T. M. Sprouse, J. Lippuner, R. Surman, A. J. Couture, P. F. Bloser, F. Shirazi, W. P. Even, W. T. Vestrand and R. S. Miller. Gamma Rays from Kilonova: A Potential Probe of r-process Nucleosynthesis. 2020. *The Astrophysical Journal*. **889** (2): 168. (LA-UR-19-24338 DOI: 10.3847/1538-4357/ab64d8)

Kunert, N., P. T. Pang, I. Tews, M. W. Coughlin and T. Dietrich. Quantifying modeling uncertainties when combining multiple gravitational-wave detections from binary neutron star sources. Submitted to *Physical Review D Letters*. (LA-UR-21-27560)

Lawson, T., M. Pignatari, R. J. Stancliffe, J. den Hartogh, S. Jones, C. L. Fryer, B. K. Gibson and M. Lugaro. Radioactive nuclei in the Early Solar System: a revision of the core-collapse supernova scenario. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-25978)

Lim, H. and A. Held. Nonlinear Dynamics of Quadratic Gravity in the Spherical Symmetry. Submitted to *Physical Review D*. (LA-UR-21-22739)

*Loiseau, J., H. Lim, M. A. Kaltenborn, O. Korobkin, C. M. Mauney, I. Sagert, W. P. Even and B. K. Bergen. FleCSPH: The next generation FleCSIble parallel computational infrastructure for smoothed particle hydrodynamics. 2020. *SoftwareX*. **12**: 100602. (LA-UR-20-23626 DOI: 10.1016/j.softx.2020.100602)

*Martin, J. D., J. Carlson, V. Cirigliano and D. Huaiyu. Fast flavor oscillations in dense neutrino media with collisions. 2021. *Physical Review D*. **103** (6): 063001. (LA-UR-20-30504 DOI: 10.1103/PhysRevD.103.063001)

Meshkhi, M. M., N. E. Wolfe, Z. Dai, C. Frohlich, J. M. Miller, R. K. W. Wong and R. Vilalta. A New Constraint on the Nuclear Equation of State from Statistical Distributions of Compact Remnants of Supernovae. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-30803)

*Miller, J. M., B. R. Ryan, J. C. Dolence, A. Burrows, C. J. Fontes, C. L. Fryer, O. Korobkin, J. Lippuner, M. R. Mumpower and R. T. Wollaeger. Full transport model of GW170817-like disk produces a blue kilonova. 2019. *Physical Review D*. **100** (2): 023008. (LA-UR-19-22623 DOI: 10.1103/PhysRevD.100.023008)

*Miller, J. M., B. R. Ryan and J. C. Dolence. : Radiation GRMHD for Neutrino-driven Accretion Flows. 2019. *The Astrophysical Journal Supplement Series*. **241** (2): 30. (LA-UR-19-20336 DOI: 10.3847/1538-4365/ab09fc)

Miller, J. M., T. M. Sprouse, C. L. Fryer, B. R. Ryan, J. C. Dolence, M. R. Mumpower and R. A. Surman. Full Transport General Relativistic Radiation Magnetohydrodynamics for Nucleosynthesis in Collapsars. Submitted to *Astrophysical Journal*. (LA-UR-19-30392)

Misch, G. W., L. Wang, L. Tan, Z. Li and Y. Sun. Urca Cooling in Neutron Star Crusts and Oceans: Effects of Nuclear Excitations. Submitted to *Physical Review Letters*. (LA-UR-21-21037)

Misch, G. W., M. R. Mumpower, T. M. Sprouse, A. J. Couture, C. L. Fryer, Y. Sun and B. S. Meyer. Sensitivity of Neutron-Rich Nuclear Isomer Behavior to Uncertainties in Direct Transitions. 2021. *Symmetry*. **13** (10): 1831. (LA-UR-21-21559 DOI: 10.3390/sym13101831)

*Misch, G. W., S. K. Ghorui, P. Banerjee, Y. Sun and M. R. Mumpower. Astromers: Nuclear Isomers in Astrophysics. 2020. *The Astrophysical Journal Supplement Series*. **252** (1): 2. (LA-UR-20-22828 DOI: 10.3847/1538-4365/abc41d)

Misch, G. W., T. M. Sprouse and M. R. Mumpower. Astromers in the radioactive decay of r-process nuclei. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-29246)

Mottola, E., P. Beltracchi and P. Gondolo. Slowly rotating gravastars. Submitted to *Physical Review D*. (LA-UR-21-22546)

Mottola, E., P. Beltracci and P. Gondolo. Surface Stress Tensor and Junction Conditions on a Rotating Null Horizon. Submitted to *Physical Review D*. (LA-UR-20-30222)

*Murphy, J. W., Q. Mabanta and J. C. Dolence. A comparison of explosion energies for simulated and observed core-collapse supernovae. 2019. *Monthly Notices of the Royal Astronomical Society*. **489** (1): 641-652. (LA-UR-19-23383 DOI: 10.1093/mnras/stz2123)

Nikas, S., G. Perdikakis, M. Beard, R. Surman, M. R. Mumpower and P. Tsintari. Propagation of Hauser-Feshbach uncertainty estimates to r-process nucleosynthesis: benchmark of statistical property models for neutron-rich nuclei far from stability. Submitted to *PRC*. (LA-UR-20-25713)

O'Conner, B., E. Troja, S. Dichiara, E. A. Chase, G. Ryan, S. Cenko, C. L. Fryer, R. Ricchi, F. Marshall, C. Kouveliotou, R. T. Wollaeger, C. J. Fontes, O. Korobkin, P. Gatkine, A.

Kutyrev, S. Veilleux, N. Kawai and T. Sakamoto. A tale of two mergers: constraints on kilonova detection in two short GRBs at z~0.5. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-28608)

Orford, R., N. Vassh, J. A. Clark, G. C. McLaughlin, M. R. Mumpower, D. Ray, G. Savard, R. Surman, F. Buchinger, D. P. Burdette, M. T. Burkey, D. A. Gorelov, J. W. Klimes, W. S. Porter, K. S. Sharma, A. A. Valverde, L. Varriano and X. L. Yan. Searching for the origin of the rare-earth peak with precision mass measurements across Ce-Eu isotopic chains. Submitted to *Physical Review Letters*. (LA-UR-21-23642)

Pang, P. T., I. Tews, T. Dietrich, M. W. Coughlin, M. Bulla and C. Van Den Broeck. Nuclear Physics Multimessenger Astrophysics Constraints on the Neutron Star Equation of State: Adding NICER's PSR J0740+6620 Measurement. Submitted to *Astrophysical Journal*. (LA-UR-21-20534)

*Reiter, M. P., S. A. San Andres, S. Nikas, J. Lippuner, C. Andreoiu, C. Babcock, B. R. Barquest, J. Bollig, T. Brunner, T. Dickel, J. Dilling, I. Dillmann, E. Dunling, G. Gwinner, L. Graham, C. Hornung, R. Klawitter, B. Kootte, A. A. Kwiatkowski, Y. Lan, D. Lascar, K. G. Leach, E. Leistenschneider, G. Martinez-Pinedo, J. E. McKay, S. F. Paul, W. R. Plass, L. Roberts, H. Schatz, C. Scheidenberger, A. Sieverding, R. Steinbrugge, R. Thompson, M. E. Wieser, C. Will and D. Welch. Mass measurements of neutron-rich gallium isotopes refine production of nuclei of the first -process abundance peak in neutron-star merger calculations. 2020. *Physical Review C*. **101** (2): 025803. (LA-UR-18-28439 DOI: 10.1103/PhysRevC.101.025803)

Ristic, M., E. Champion, R. O'Shaugnessy, R. T. Wollaeger, O. Korobkin, E. A. Chase, C. L. Fryer, A. L. Hungerford and C. J. Fontes. Interpolating detailed simulations of kilonovae: adaptive learning and parameter inference applications. Submitted to *Astrophysical Journal*. (LA-UR-21-24289)

Riz, L., F. Pederiva, D. Lonardoni and S. Gandolfi. Spin susceptibility in neutron matter from quantum Monte Carlo calculations. Submitted to *Particles*. (LA-UR-20-28566)

L. Rosa, J. D., P. Roming and C. L. Fryer. Finding Shock Breakout. Submitted to *Astrophysical Journal*. (LA-UR-19-30389)

Ruiz-Lapuente, M. P. and O. Korobkin. Gamma-rays from kilonovae and the cosmic gamma-ray background. Submitted to *Astrophysical Journal*. (LA-UR-20-20301)

Safi-Harb, S., N. Doerksen, A. Rogers and C. L. Fryer. Chandra X-ray Observations of the Neutron Star Merger GW170817: Evidence of Thermal X-ray Emission. Submitted to *Journal of the Royal Astronomy Society of Canada*. (LA-UR-18-30639)

Salvesen, G. M. and J. M. Miller. Black Hole Spin in X-ray Binaries: Giving Uncertainties an f. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-28487)

*Setzer, C. N., R. Biswas, H. V. Peiris, S. Rosswog, O. Korobkin and R. T. Wollaeger. Serendipitous discoveries of kilonovae

in the LSST main survey: maximizing detections of sub-threshold gravitational wave events. 2019. *Monthly Notices of the Royal Astronomical Society*. **485** (3): 4260-4273. (LA-UR-18-31553 DOI: 10.1093/mnras/stz506)

Somasundaram, R., I. Tews and J. Margueron. Astrophysical Constraints on the Sound-Speed Profile in Dense Matter. Submitted to *Physical Review C*. (LA-UR-21-22340)

*M. M. *. S. R. Sprouse, T. *., T. M. Sprouse and M. R. Mumpower. Following Fission Products in Explosive Astrophysical Environments. *EPJ Web of Conferences*. **242**: 4001. (LA-UR-20-21940 DOI: 10.1051/epjconf/202024204001)

. M. M. R. *. S. R. Sprouse, T. M., T. M. Sprouse and M. R. Mumpower. Following nuclei through nucleosynthesis: A novel tracing technique. 2021. *Physical Review C*. **104 (1): 015803. (LA-UR-20-24018 DOI: 10.1103/PhysRevC.104.015803)

Sprouse, T. M., G. W. Misch and M. R. Mumpower. Isochronic evolution and the radioactive decay of r-process nuclei. Submitted to *Astrophysical Journal. Supplement Series*. (LA-UR-21-20819)

Sundermann, R., H. Lim, J. Waybright and J. Kimn. A Spacetime Finite Element Method to Solve the Dirac Equation. Submitted to *Journal of Computational Physics*. (LA-UR-21-22066)

Tews, I., D. Lonardoni and S. Gandolfi. Chiral Effective Field Theory's Impact in AdvancingQuantum Monte Carlo Methods. Submitted to *Few-Body Systems Special Issue "Celebrating 30 years of the Steven Weinberg's paper Nuclear Forces from Chiral Lagrangians"*. (LA-UR-21-28301)

Thakur, A. L., S. Dichiara, E. Troja, E. A. Chase, R. Sanchez-Ramirez, L. Piro, C. L. Fryer, N. R. Butler, R. T. Wollaeger, E. Ambrosi, J. Becerra Gonzalez, R. L. Becerra, G. Bruni, B. S. Cenko, G. Cusumano, A. D'Ai, J. Durbak, C. J. Fontes, P. Gatkine, A. L. Hungerford, O. Korobkin, A. S. Kutyrev, W. H. Lee, S. Lotti, G. Minervini, G. Novara, V. La Parola, M. Pereyra, R. Ricci, A. Tiengo, S. Veilleux and A. M. Watson. A search for optical and near-infrared counterparts of the candidate neutron star - black hole merger GW190814. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-24948)

*Vance, G. S., P. A. Young, C. L. Fryer and C. I. Ellinger. Titanium and Iron in the Cassiopeia A Supernova Remnant. 2020. *The Astrophysical Journal*. **895** (2): 82. (LA-UR-19-24919 DOI: 10.3847/1538-4357/ab8ade)

Wang, X., B. D. Fields, M. R. Mumpower, T. M. Sprouse, R. Surman and N. Vassh. Sandblasting the r-process: spallation of ejecta from neutron star mergers. Submitted to *Astrophysical Journal*. (LA-UR-19-29391)

Wang, X., N. Vassh, T. M. Sprouse, M. R. Mumpower, R. Vogt, J. Randrup and R. Surman. MeV gamma-rays from fission: a unique signature of actinide production in neutron star

mergers. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-25892)

White, N., F. Bauer, W. Baumgartner, M. Bautz, E. Berger, S. B. Cenko, T. Chang, A. Falcone, H. Fausey, C. Feldman, D. Fox, O. Fox, A. Fruchter, C. L. Fryer, G. Ghirlanda, K. Gorski, K. Grant, S. Guiriec, M. Hart, D. Hartmann, J. Hennawi, D. A. Kann, D. Kaplan, J. A. Kennea, D. Kocevski, C. Kouveliotou, C. Lawrence, A. J. Levan, A. Lidz, A. Lien, T. B. Littenberg, L. Mas-Ribas, M. Moss, P. O'Brien, J. O'Meara, D. Palmer, D. Pasham, J. Racusin, R. Remillard, O. Roberts, P. Roming, M. Rud, R. Salvaterra, R. Sambruna, M. Seiffert, G. Sun, N. R. Tanvir, R. Terrile, N. Thomas, A. J. Van Der Horst, W. T. Vestrand, P. Willems, C. A. Wilson-Hodge, E. T. Young, L. Amati, E. Bozzo, O. L. Karczewski, C. Hernandez-Monteagudoa, R. Rebolo Lopez, R. Genova-Santos, A. Martin, J. Granot, P. Bemiamini, R. Gil and E. Burns. The Gamow Explorer: A gamma-ray burst observatory to study the high redshift universe and enable multi-messenger astrophysics. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-21-31435)

*Wollaeger, R. T., C. L. Fryer, C. J. Fontes, J. Lippuner, W. T. Vestrand, M. R. Mumpower, O. Korobkin, A. L. Hungerford and W. P. Even. Impact of Pulsar and Fallback Sources on Multifrequency Kilonova Models. 2019. *The Astrophysical Journal*. **880** (1): 22. (LA-UR-19-22590 DOI: 10.3847/1538-4357/ab25f5)

Wollaeger, R. T., C. L. Fryer, E. A. Chase, C. J. Fontes, M. Ristic, A. L. Hungerford, O. Korobkin, R. O'Shaughnessy and A. M. Herring. A Broad Grid of 2D Kilonova Emission Models. Submitted to *Astrophysical Journal*. (LA-UR-20-30338)

*Wu, J., S. Nishimura, P. Moller, M. R. Mumpower, R. Lozeva, C. B. Moon, A. Odahara, H. Baba, F. Browne, R. Daido, P. Doornenbal, Y. F. Fang, M. Haroon, T. Isobe, H. S. Jung, G. Lorusso, B. Moon, Z. Patel, S. Rice, H. Sakurai, Y. Shimizu, L. Sinclair, P. A. Soderstrom, T. Sumikama, H. Watanabe, Z. Y. Xu, A. Yagi, R. Yokoyama, D. S. Ahn, F. L. Bello Garrote, J. M. Daugas, F. Didierjean, N. Fukuda, N. Inabe, T. Ishigaki, D. Kameda, I. Korjouharov, T. Komatsubara, T. Kubo, T. Kurz, K. Y. Kwon, S. Morimoto, D. Murai, H. Nishibata, H. Schaffner, T. M. Sprouse, H. Suzuki, H. Takeda, M. Tanaka, K. Tshoo and Y. Wakabayashi. -decay half-lives of 55 neutron-rich isotopes beyond the shell gap. 2020. *Physical Review C*. **101** (4): 042801. (LA-UR-20-22956 DOI: 10.1103/PhysRevC.101.042801)

Conference Papers

Fryer, C. L., A. L. Hungerford and S. Jones. Gamma-Ray Probes of Supernova Engines. Presented at *12th Integral Conference*. (Geneva, Switzerland, 2019-02-11 - 2019-02-15). (LA-UR-19-23463)

Fryer, C. L., C. J. Fontes, O. Korobkin, M. R. Mumpower, R. T. Wollaeger, E. Holmbeck and R. O'Shaugnessy. Uncertainties in Kilonova Modeling. Presented at *Marcel Grossmann*

16. (Virtual meeting, Italy, 2021-07-05 - 2021-07-10). (LA-UR-21-30201)

Holmbeck, E., R. Surman, A. Frebel, G. C. McLaughlin, M. R. Mumpower, T. M. Sprouse, T. Kawano, N. Vassh and T. C. Beers. Characterizing r-process sites through actinide production. Presented at *Nuclear Physics in Astrophysics IX*. (Frankfurt, Germany, 2019-09-15 - 2019-09-15). (LA-UR-20-22074)

Korobkin, O., H. Lim, J. Loiseau, C. M. Mauney, I. Sagert, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *Spheric 2021*. (Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11). (LA-UR-21-24198)

Mumpower, M. R., M. Verriere and J. Randrup. Fission yields using a macroscopic-microscopic model. Presented at *Compound Nuclear Reactions*. (Athens, Greece, 2020-10-05 - 2020-10-05). (LA-UR-20-23188)

Stewart, A. R., L. Lo, O. Korobkin, J. Loiseau, H. Lim, M. A. R. Kaltenborn and C. M. Mauney. Realistic Kilonova Up Close. Presented at *SuperComputing 2021 (SC21): SciViz Showcase*. (St. Louis, Missouri, United States, 2021-11-17 - 2021-11-17). (LA-UR-21-28322)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *Spheric 2021*. (Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11). (LA-UR-21-24191)

Reports

Allen, G., I. Andreoni, E. Bachelet, B. Berriman, R. Biswas, D. George, W. Gropp, A. Gupta, R. Haas, E. Huerta, E. Jennings, D. Katz, A. Khan, V. Kindratenko, W. T. C. Kramer, A. Mahabal, J. M. Miller, A. Olivas, M. Ruiz, A. Saxton, E. Seidel, S. Shapiro, H. Shen, L. Sun, J. Towns, A. Tsokaros, W. Wei and Z. Zhao. Deep Learning for Multi-Messenger Astrophysics: A Gateway for Discovery in the Big Data Era. Unpublished report. (LA-UR-19-21084)

Burns, E., A. Tohuvavohu, C. Wilson-Hodge, D. Eichler, C. L. Fryer, J. Buckley, D. Radice, B. D. Metzger, B. Zhang, K. Murase, J. Tomsick and T. Dal Canton. A Summary of Multimessenger Science with Neutron Star Mergers. Unpublished report. (LA-UR-19-21845)

Burns, E., A. Tohuvavohu, J. Bellovary, E. Blaufuss, T. Brandt, S. Buson, R. Caputo, S. B. Cenko, N. Christensen, J. Conklin, F. D'Ammando, K. Ford, A. Franckowiak, C. L. Fryer, K. Holley-Bockelmann, T. Jaffe, T. Kupfer, M. Karovska, B. Metzger, J. Racusin, B. Rani, M. Santander, J. Tomsick and C. Wilson-Hodge. Opportunities for Multimessenger Astronomy in the 2020s. Unpublished report. (LA-UR-19-22226)

Burns, E., S. Zhu, C. Hui, S. Ansoldi, S. Barthelmy, S. Boggs, S. Cenko, N. Christensen, C. L. Fryer, A. Goldstein, A. Harding, D. Hartmann, A. Joens, G. Kanbach, M. Kerr, C. Kierans,

J. McEnery, B. Patricelli, J. Perkins, J. Racusin, P. Ray, J. Schleider, H. Schoorlemmer, F. Schussler, J. Slutsky, A. Stamerra, J. Tomsick, Z. Wadiasingh, C. Wilson-Hodge, G. Younes and A. Zoglauer. Gamma Rays and Gravitational Waves. Unpublished report. (LA-UR-19-22122)

Chatziioannou, K., W. R. Hix, P. Landry, W. Lynch, D. Radice, L. Roberts, A. Steiner, I. Tews and A. Watts. JINA Horizons White Paper, Dense Matter Working Group. Unpublished report. (LA-UR-21-24945)

Couture, A. J., L. Nies, K. Blaum, R. B. Cakirli, R. F. Casten, W. J. Huang, J. Karthein, I. Kulikov, Y. A. Litvinov, D. Lunney, V. Manea, G. W. Misch, M. Mougeot, M. R. Mumpower, C. J. Prokop, L. Schweikhard and F. Wienholtz. Measurement of the excitation of the 5+ isomer energy in128Sb for r-process nucleosynthesis. Unpublished report. (LA-UR-21-24380)

Couture, A. J., L. Nies, K. Blaum, R. B. Cakirli, R. F. Casten, W. J. Huang, J. Karthein, I. Kulikov, Y. A. Litvinov, D. Lunney, V. Manea, G. W. Misch, M. Mougeot, M. R. Mumpower, C. J. Prokop, L. Schweikhard and F. Wienholtz. Measurement of the excitation of the 5+ isomer energy in128Sb for r-process nucleosynthesis. Unpublished report. (LA-UR-21-24380)

Foley, R. J., K. D. Alexander, I. Andreoni, I. Arcavi, K. Auchettl, G. Baym, E. C. Bellm, J. P. Blakeslee, P. R. Brady, M. Branchesi, J. S. Brown, R. Chornock, J. Cooke, A. Corsi, M. W. Coughlin, D. A. Coulter, P. S. Cowperthwaite, G. Dimitriadis, M. R. Drout, R. Fernandez, A. V. Filippenko, W. Fong, D. A. Frail, W. L. Freedman, C. L. Fryer, V. Z. Golkhou, D. Hiramatsu, G. Hosseinzadeh, K. Hotokezaka, D. A. Howell, T. Hung, D. O. Jones, V. Kalogera, D. Kasen, W. E. Kerzendorf, C. D. Kilpatrick, R. P. Kirshner, J. M. Lattimer, I. Mandel, K. S. Mandel, B. Margalit, R. Margutti, J. McIver, B. D. Metzger, T. Moriya, G. Narayan, S. Nissanke, J. M. O'Meara, R. O'Shaughnessy, E. O'Connor, A. Palmese, Y. C. Pan, C. Pankow, K. Paterson, D. A. Perley, R. Perna, A. L. Piro, T. A. Pritchard, E. Quataert, D. Radice, E. Ramirez-Ruiz, S. Reddy, A. Rest, A. G. Riess, C. Rojas-Bravo, S. Rosswog, M. Ruiz, S. L. Shapiro, M. R. Siebert, D. M. Siegel, K. Siellez, N. Smith, M. Soares-Santos, N. B. Suntzeff, M. Tanaka, N. R. Tanvir, G. Terreran, S. Valenti, S. A. Webb, J. C. Wheeler, S. Woosley, M. Zaldarriaga and M. Zevin. Gravity and Light: Combining Gravitational Wave and Electromagnetic Observations in the 2020s. Unpublished report. (LA-UR-19-22283)

Frontera, F., E. Virgilli, C. Guidorzi, P. Rosati, R. Diehl, T. Siegert, C. L. Fryer, L. Amati, N. Auricchio, R. Campana, E. Caroli, F. Fuschino, C. Labanti, M. Orlandini, E. Pian, J. Stephen, S. Del Sordo, C. Budtz-Jorgensen, I. Kuvvetli, S. Brandt, R. Curado de Silva, P. Laurent, P. Mazzali and M. Della Valle. Understanding the origin of the positron annihilation line and the physics of supernova explosions. Unpublished report. (LA-UR-19-27793)

Fryer, C. L., E. Burns, P. W. Roming, P. Slane, M. Szczepanczyk, I. Tomborra and R. Trappitsch. Core-Collapse Supernovae and Multi-Messenger Astronomy. Unpublished report. (LA-UR-19-22444)

Guirec, S., J. Tomsick, D. Hartmann, T. Brandt, M. Ajello, A. De Angelis, E. Bissaldi, B. Rani, Z. Wadiasingh, F. Timmes, A. van der Horst, F. D'Ammando, M. Petropoulou, V. Tatischeff, T. Venters, R. Walter, B. Zhang, R. Ojha, C. L. Fryer and X. Wang. Gamma-Ray Science in the 2020s. Unpublished report. (LA-UR-19-22230)

Kierans, C., S. Boggs, M. Buckley, R. Caputo, R. Crocker, M. De Becker, R. Diehl, C. L. Fryer, S. Griffin, D. Hartmann, E. Hays, P. Jean, M. Krause, T. Linden, P. Martin, A. Moiseev, U. Oberlack, F. Panther, N. Prantzos, R. Rothschild, I. Seitenzahl, C. Shrader, T. Siegert, J. Tomsick and A. Zoglauer. Positron Annihilation in the Galaxy. Unpublished report. (LA-UR-19-22191)

Kolos, K., G. Savard, G. W. Misch, M. R. Mumpower, R. Orford, M. Bencomo, N. Scielzo, J. A. Clark, D. E. M. Hoff, G. Kondev, W. J. Ong, D. Ray, D. Santiago-Gonzalez, A. A. Valverde and X. Yan. Measurements of Isomer Energies in Potential "Astromers". Unpublished report. (LA-UR-21-22190)

Korobkin, O. Institutional Computing 2019/2020 Project Report: First Year. Unpublished report. (LA-UR-20-25524)

Korobkin, O. Institutional Computing 2019/2020 Allocation Report: Viewgraphs, Year 1. Unpublished report. (LA-UR-20-25615)

Kupfer, T., M. Kilic, T. Maccarone, E. Burns and C. L. Fryer. A Summary of Multimessenger Science with Galactic Binaries. Unpublished report. (LA-UR-19-22243)

Lim, H. Dynamics of Compact Objects in Numerical Relativity. Unpublished report. (LA-UR-19-27066)

Lim, H. FleCSPH Wiki. Unpublished report. (LA-UR-20-26581)

Miller, J. M. w19_nubhlight Report. Unpublished report. (LA-UR-20-21905)

Miller, R., M. Ajello, J. Beacom, P. F. Bloser, A. Burrows, C. L. Fryer, J. Goldsten, D. Hartmann, P. Hoeflich, A. L. Hungerford, D. Lawrence, M. Leising, P. A. Milne, P. Peplowski, F. Shirazi, T. Sukhbold, L. The, Z. Yokley and C. Young. Ex Luna, Scientia: The Lunar Occultation eXplorer (LOX). Unpublished report. (LA-UR-19-26900)

Mumpower, M. R., O. Korobkin, J. M. Miller and T. M. Sprouse. Nuclear Data for Astrophysics on the Eve of FRIB. Unpublished report. (LA-UR-20-26586)

Tomsick, J. A., A. Zoglauer, C. Sleator, L. Hadar, J. Beechert, S. Boggs, J. Roberts, T. Siegert, A. Lowell, E. Wulf, B. Philips, T. Brandt, A. Smale, C. Kierans, E. Burns, D. Hartmann, M. Leising, M. Ajello, C. L. Fryer, M. Amman, H. Chang, P. Jean and P. von Ballmoos. Astro 2020 APC White Paper: The Compton Spectrometer and Imager. Unpublished report. (LA-UR-19-26922)

Zingale, M., C. L. Fryer, A. L. Hungerford, S. Safi-Harb, R. Trappitsch, R. A. Fisher, A. Calder and K. J. Shen. MMA SAG: Thermonuclear Supernovae. Unpublished report. (LA-UR-19-22421)

Presentation Slides

Couture, A. J. CENTAUR Highlight: LANL Collaboration. Presented at *CENTAUR First Year Review*, College Station, Texas, United States, 2019-03-11 - 2019-03-11. (LA-UR-19-22538)

Couture, A. J., R. F. Casten and R. B. Cakirli. Nuclear Masses, Neutron Capture, and the r Process. Presented at *Division of Nuclear Physics, American Physical Society Fall Meeting*, Arlington, Virginia, United States, 2019-10-15 - 2019-10-15. (LA-UR-19-30684)

Dolence, J. C. Full Transport GR Neutrino Radiation MHD and Nucleosynthesis in Neutron Star Merger Disks. Presented at *Explosive Nucleosynthesis in the Supernova and Merging-Neutron-Star Contexts*, Princeton, New Jersey, United States, 2019-05-22 - 2019-05-24. (LA-UR-19-24793)

Dolence, J. C. Frontiers of Relativistic Radiation Magnetohydrodynamics. Presented at *APS April Meeting: Quarks to Cosmos*, College Park, Maryland, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23716)

Even, W. P. Searching For The Origin Of Gold In The Universe. . (LA-UR-20-29377)

Even, W. P. The Origin Of Heavy Elements In The Universe. . (LA-UR-21-21837)

Fontes, C. J. Atomic Physics and the Spectral Modeling of Kilonovae. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, online, New Mexico, United States, 2021-05-31 - 2021-06-04. (LA-UR-21-25299)

Fontes, C. J., C. L. Fryer, A. L. Hungerford, R. T. Wollaeger and O. Korobkin. A Link between Atomic Physics and Gravitational Wave Spectroscopy. Presented at *20th International Conference on Atomic Processes in Plasmas*, Gaithersburg, Maryland, United States, 2019-04-08 - 2019-04-12. (LA-UR-19-23290)

Fryer, C. L. Nucleosynthesis Probes of Cosmic Explosions: Understanding Neutron Star Mergers. . (LA-UR-20-29858)

Fryer, C. L. Physics Behind Cosmic Explosions. . (LA-UR-21-25869)

Fryer, C. L. Uncertainties in Modeling Kilonova Emission. Presented at *16th Marcel Grossman Conference*, Virtual meeting, Italy, 2021-07-05 - 2021-07-10. (LA-UR-21-26127)

Fryer, C. L. Probes of the Progenitors, Engines and Physics behind Stellar Collapse. Presented at *16th Marcel Grossmann conference*, Virtual meeting, Italy, 2021-07-05 - 2021-07-10. (LA-UR-21-26119)

Fryer, C. L., S. Gandolfi, P. R. Wozniak, J. A. Carlson, A. J. Couture, J. C. Dolence, W. P. Even, C. J. Fontes, A. L. Hungerford, O. Korobkin, J. M. Miller, G. W. Misch, E. Mottola, M. R. Mumpower, J. Lippuner, W. T. Vestrand and R. T. Wollaeger. Nucleosynthesis Probes of Cosmic Explosions. . (LA-UR-20-22078)

Guzik, J. A., E. K. Farag, J. Ostrowski, N. Evans, H. Neilson, S. Moschou and J. Drake. Modeling Cepheid Variable Stars Using the Open-Source MESA Code. Presented at *AAVSO 108th Annual Meeting*, Las Cruces, New Mexico, United States, 2019-10-18 - 2019-10-20. (LA-UR-19-30082)

Guzik, J. A., E. K. Farag, J. Ostrowski, N. Evans, H. Neilson, S. Moschou and J. Drake. Investigating Opacity Modifications and Reaction Rate Uncertainties to Resolve the Cepheid Mass Discrepancy. Presented at *RRL/Cep 2019--Frontiers of Classical Pulsators: Theory and Observations*, Cloudcroft, New Mexico, United States, 2019-10-13 - 2019-10-18. (LA-UR-19-30239)

Hungerford, A. L. Astrophysical Radionuclides: where are they and what can they tell us?. Presented at *KITP: The new era of gravitational wave astronomy*, Santa Barbara, California, United States, 2019-06-24 - 2019-07-19. (LA-UR-19-26062)

R. Kaltenborn, M. A., W. P. Even, O. Korobkin, H. Lim, J. Loiseau, C. M. Mauney and I. Sagert. FleCSPH for Modeling Binary White Dwarf Mergers. Presented at *The 37th Annual New Mexico Symposium*, Los Alamos, New Mexico, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31301)

R. Kaltenborn, M. A., W. P. Even, O. Korobkin, H. Lim, J. Loiseau, C. M. Mauney and I. Sagert. FleCSPH for Modeling Binary White Dwarf Mergers. Presented at *The 37th Annual New Mexico Symposium*, Los Alamos, New Mexico, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31373)

R. Kaltenborn, M. A., W. P. Even, O. Korobkin, H. Lim, J. Loiseau, C. M. Mauney and I. Sagert. FleCSPH for Modeling Compact Merger Binaries and Accretion Disk Remnants. Presented at *239th Meeting of the American Astronomical Society*, Salt Lake City, Utah, United States, 2022-01-09 - 2022-01-09. (LA-UR-21-32334)

Korobkin, O. Mergers of Compact Objects with SPH and General Relativity, Institutional Computing Allocation Report: Year 2. . (LA-UR-19-22138)

Korobkin, O. Radioactivity gamma-rays in the aftermath of neutron star mergers: a probe of the r-process nucleosynthesis. Presented at *R-Process Alliance Workshop: Pushing toward the Next Project Phases*, Cambridge, Massachusetts, United States, 2019-11-20 - 2019-11-22. (LA-UR-19-31907)

Korobkin, O., R. T. Wollaeger, C. L. Fryer, A. L. Hungerford, E. A. Chase, S. Rosswog, C. J. Fontes, M. R. Mumpower, W. P. Even, J. M. Miller, G. W. Misch and J. Lippuner. Multidimensional Radiative Transfer Models of Kilonovae. Presented at *APS April Meeting*, Online meeting, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-24013)

Lim, H. Safe Travel Guide to Black Hole. . (LA-UR-20-22133)

Lim, H. Are we alone? Searching Intelligent Life Beyond the Earth. . (LA-UR-20-25542)

Lim, H. What's Up Gravitational Waves! More Messages from Ripples of Spacetime. . (LA-UR-20-29295)

Lim, H. Nonlinear Dynamics of Modified Gravity Theories. . (LA-UR-20-29857)

Lim, H. Nonlinear Dynamics of Beyond General Relativity : Strong Field Regime with Gravitational Waves. . (LA-UR-21-28685)

Lim, H., O. Korobkin, J. Loiseau, C. M. Mauney, I. Sagert, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *Spheric 2021*, Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25052)

Lim, H., O. Korobkin, J. Loiseau, C. M. Mauney, I. Sagert, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *Spheric 2021*, Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25190)

Lippuner, J. The origin of heavy elements. . (LA-UR-18-30723)

Lippuner, J. r-Process nucleosynthesis and kilonova overview. Presented at *12th INTEGRAL Conference*, Geneva, Switzerland, 2019-02-11 - 2019-02-15. (LA-UR-19-20935)

Lippuner, J. r-Process nucleosynthesis and kilonovae from neutron star mergers. Presented at *Multi-Messenger Astrophysics in the Gravitational Wave Era*, Kyoto, Japan, 2019-09-30 - 2019-10-04. (LA-UR-19-29973)

Lippuner, J. Nuclear Network Calculations of Kilonova Ejecta. Presented at *APS April Meeting 2021*, Virtual, Missouri, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-23672)

Lo, L., A. R. Stewart, O. Korobkin and J. Loiseau. Visualization of a Neutron Star Binary Merger and Subsequent Creation of Kilonova. Presented at *Supercomputing Conference 2021*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14. (LA-UR-21-27889)

Loisel, G. P., J. E. Bailey, S. B. Hansen, T. Nagayama, G. A. Rochau, E. Harding, D. A. Liedahl, C. J. Fontes, R. C. Mancini and T. R. Kallman. A benchmark Experiment for X-ray Emission and Temperature Diagnostics in Accretion-Powered Photoionized Plasmas. Presented at *20th International Conference on Atomic Processes in Plasmas*, Gaithersburg, Maryland, United States, 2019-04-09 - 2019-04-12. (LA-UR-19-24480)

Miller, J. M. No Return: What are black holes and how do we see them?. . (LA-UR-19-31121)

Miller, J. M. Why We Need (But Don't have) Quantum Gravity. . (LA-UR-19-31190)

Miller, J. M. Outflow from a post-neutron star merger disk. . (LA-UR-20-21906)

Miller, J. M. A Universe of Unknowns: Dark Matter and Dark Energy. . (LA-UR-20-21904)

Miller, J. M. Neutrinos: The Ghosts From Space. . (LA-UR-20-26425)

Miller, J. M. Challenges and Opportunities in Post-Merger Disks. Presented at *Mathematical and Computational Approaches for the Einstein Field Equations with Matter Fields*, Los Alamos, New Mexico, United States, 2020-10-26 - 2020-10-30. (LA-UR-20-28707)

Miller, J. M. Mining for Cosmic Gold with Supercomputers. . (LA-UR-20-29615)

Miller, J. M. End-to-End Modeling of a Kilonova. Presented at *238th Meeting of the AAS/LAD*, Los Alamos, New Mexico, New Mexico, United States, 2021-06-07 - 2021-06-09. (LA-UR-21-25239)

Miller, J. M. End-to-End Modeling of a Kilonova. . (LA-UR-21-28556)

Miller, J. M., B. R. Ryan, J. C. Dolence, A. Burrows, C. L. Fryer, J. Lippuner and M. R. Mumpower. Fusion in Space: Nuclear Astrophysics, Neutron Star Mergers, and Accretion Disks. Presented at *Arizona-Los Alamos Days*, Tuscon, Arizona, United States, 2019-04-19 - 2019-04-21. (LA-UR-19-23149)

Miller, J. M., B. R. Ryan, J. C. Dolence, A. Burrows, C. L. Fryer, J. Lippuner and M. R. Mumpower. Neutrino GRRMHD for Neutron Star Merger Disks with bhlight: Models and Implications. Presented at *TCAN 2019*, Princeton, New Jersey, United States, 2019-04-13 - 2019-04-17. (LA-UR-19-23214)

Miller, J. M., C. L. Fryer, M. R. Mumpower and R. A. Surman. Astrophysics Uncertainties in Kilonova Modeling. Presented at *FRIB First Experiments Workshop*, Online, New Mexico, United States, 2020-05-04 - 2020-05-08. (LA-UR-20-23436)

Miller, J. M., T. M. Sprouse, C. L. Fryer, B. R. Ryan, J. C. Dolence, R. A. Surman and M. R. Mumpower. Neutrino Transport and Nucleosynthesis in Collapsars. Presented at *SciDAC TEAMS collaboration meeting*, Los Alamos, New Mexico, United States, 2020-06-15 - 2020-06-16. (LA-UR-20-24494)

Miller, J. M., T. M. Sprouse, S. Curtis and S. De. Neutrino Transport and Nucleosynthesis in Post-Merger Disks. . (LA-UR-20-30341)

Miller, J. M., T. M. Sprouse and C. L. Fryer. Neutrino Transport and Nucleosynthesis in Collapsars. Presented at *LANL UA Days*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-19. (LA-UR-20-23437)

Miller, J. M. and P. Polko. Black Holes I. . (LA-UR-19-23242)

Misch, G. W. Neutrinos from Pre-supernova Stars. Presented at *Invited talk at University of Notre Dame*, North Bend, Indiana, United States, 2019-09-10 - 2019-09-10. (LA-UR-19-30458)

Misch, G. W. Astromers: Nuclear Isomers with Astrophysical Consequences. . (LA-UR-21-21516)

Misch, G. W., M. R. Mumpower, Y. Sun, S. K. Ghorui and P. Banerjee. Astromers: Nuclear Isomers with Astrophysical Consequences. . (LA-UR-20-26202)

Misch, G. W., M. R. Mumpower and C. W. Johnson. Nuclear Shell Model Calculations for Astrophysical Weak Interactions. . (LA-UR-21-23485)

Mumpower, M. R. Fission properties for r-process nucleosynthesis. Presented at *ASU r-process workshop*, Tempe, Arizona, United States, 2019-03-26 - 2019-03-30. (LA-UR-19-22694)

Mumpower, M. R. Astrophysical aspects of r-process nucleosynthesis in neutron star mergers. Presented at *Astrophysics seminar*, South Bend, Indiana, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-24076)

Mumpower, M. R. Nucleosynthesis: connecting nuclear physics to astrophysics. Presented at *Frontiers summer school*, Lansing, Michigan, United States, 2019-05-14 - 2019-05-18. (LA-UR-19-24624)

Mumpower, M. R. Overlap of nuclear physics and nucleosynthesis. Presented at *FRIB first experiments*, Los Alamos, New Mexico, United States, 2020-05-04 - 2020-05-04. (LA-UR-20-23383)

Mumpower, M. R. Probing Nuclear Physics with Neutron Star Mergers. Presented at *ECT* workshop*, Trento, Italy, 2021-07-12 - 2021-07-12. (LA-UR-20-30211)

Mumpower, M. R. Signatures of radioactive isotopes in the r-process. Presented at *Radionuclides workshop*, Los Alamos, New Mexico, United States, 2021-10-04 - 2021-10-22. (LA-UR-21-30370)

Rassel, M. N., N. M. Lloyd Ronning, P. F. H. Kilian and C. L. Fryer. Kilonova Emission - Particle-In-Cell Simulations of Mildly Relativistic Outflows. Presented at *NMAS*, albuquerque, New Mexico, United States, 2019-11-02 - 2019-11-02. (LA-UR-19-31081)

Sagert, I. and O. Korobkin. Studying Crust-Breaking Events in Neutron Stars with Strength and Smoothed Particle Hydrodynamics. . (LA-UR-20-21887)

Stewart, A. R., L. Lo, O. Korobkin, I. Sagert, J. Loiseau, H. Lim, M. A. R. Kaltenborn, C. M. Mauney and J. M. Miller. Visualization of a Neutron Star Binary Merger and Subsequent Creation of Kilonova. Presented at *Supercomputing 2021*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14. (LA-UR-21-28564)

Tews, I. The nuclear equation of state. . (LA-UR-20-30076)

Tews, I. From nuclei to neutron stars: Combining nuclear physics and multi-messenger observations. . (LA-UR-21-23345)

Tews, I. Nuclear-Physics Predictions for the Equation of State of Neutron Stars. Presented at *APS April Meeting*, Los Alamos, New Mexico, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-23490)

Tews, I. Quantum Monte Carlo Methods with chiral EFT Interactions as a consistent Approach to Nuclei and Neutron Stars. . (LA-UR-21-28640)

Tews, I. From nuclei to neutron stars: Combining nuclear physics and multi-messenger observations. . (LA-UR-21-28641)

Tews, I. From Nuclei to Neutron Stars: Combining Nuclear Physics and Multi-Messenger Observations. Presented at *2021 Fall Meeting of the APS Division of Nuclear Physics (online)*, online, New Mexico, United States, 2021-10-11 - 2021-10-14. (LA-UR-21-29984)

Tews, I. From nuclei to neutron stars: Combining nuclear physics and multimessenger observations. . (LA-UR-21-31977)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *SPHERIC 2021*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25313)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *SPHERIC 2021*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25319)

Wollaeger, R. T. SuperNu Tutorial, Part 1 Equations, Assumptions, & Discretizations. Presented at *LSU 2018*, Baton Rouge, Louisiana, United States, 2018-10-08 - 2018-10-10. (LA-UR-18-29596)

Wollaeger, R. T. Type Ia Supernova Transient Simulation Data for MPA Workshop. Presented at *Radiative transfer in supernovae*, Garching (by Munich), Germany, 2019-08-05 - 2019-08-09. (LA-UR-19-27767)

Wollaeger, R. T. Kilonova Model Grid from Multigroup Radiative Transfer in 2D Axisymmetry. Presented at *Los Alamos - Arizona Days*, Los Alamos, New Mexico, United States, 2020-05-18 - 2020-05-19. (LA-UR-20-23700)

Wollaeger, R. T. Light Curves and Spectra from Kilonova Models. . (LA-UR-21-23680)

Wollaeger, R. T. Modeling Kilonova Light-Curves. Presented at *APS April Meeting*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23735)

Posters

Fromm, S. and O. Korobkin. Exploring General Relativistic Hydrodynamics with Particle Methods. Presented at *DOE Computational Science Graduate Fellowship Program Review*, Arlington, Virginia, United States, 2019-07-15 - 2019-07-18. (LA-UR-19-26423)

Fryer, C. L., C. Ellinger, B. W. Grefenstette, A. L. Hungerford, S. Jones, O. Korobkin, G. W. Misch, M. R. Mumpower, S. Safi-Harb, G. Vance and P. Young. Radioactive Isotopes as Probes of Astrophysical Transients. Presented at *Supernova Remnants II*, Heraklion, Crete, Greece, 2019-06-03 - 2019-06-08. (LA-UR-19-24402)

Lim, H., J. Loiseau, O. Korobkin, I. Sagert, W. P. Even and B. K. Bergen. FleCSPH : A Parallel Distributed Smoothed Particle Hydrodynamics Implementation to Study Binary Compact Object Coalescence. Presented at *2019 Sandia National*

Laboratory Postdoc showcase, Albuquerque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-31667)

Lim, H., O. Korobkin, J. M. Miller, R. T. Wollaeger, C. J. Fontes, M. A. R. Kaltenborn, W. P. Even and J. Loiseau. Studying Expansion of Ejecta from Binary Neutron Star Mergers. Presented at *Aps April Meeting 2021*, Virtually Anywhere, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23238)

Miller, J. M., B. R. Ryan, J. C. Dolence, A. Burrows, C. L. Fryer, O. Korobkin, J. Lippuner, M. R. Mumpower and R. T. Wollaeger. GW170817-Like Disk Produces a Blue Kilonova. . (LA-UR-19-24475)

Rassel, M. N., P. F. H. Kilian, C. L. Fryer, N. M. Ronning, C. Huang and F. Fraschetti. Particle In Cell Simulations of Mildly Relativistic Outflows In Kilonova Emissions. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-31422)

Other

Curtis, S. and J. M. Miller. Broadband Light Curves and Spectra for a Suite of Core-Collapse Supernovae. Dataset. (LA-UR-21-24547)

Even, W. P. Type Ia Supernova xRAGE Simulation Data for MPA Workshop. Dataset. (LA-UR-19-27753)

Fontes, C. J., C. L. Fryer, A. L. Hungerford, R. T. Wollaeger and O. Korobkin. Lanthanide and Actinide Opacities for Kilonova Modeling. Dataset. (LA-UR-20-27915)

Fontes, C. J., C. L. Fryer, W. P. Even, O. Korobkin and R. T. Wollaeger. Kilonova models data. Dataset. (LA-UR-19-22878)

Fryer, C. L., W. P. Even, S. Jones and S. J. Andrews. Nucleosynthetic Yields from Core-Collapse Supernovae. Dataset. (LA-UR-19-28686)

Korobkin, O., R. T. Wollaeger, W. P. Even, C. J. Fontes and C. L. Fryer. Axisymmetric kilonova models: dataset release. Dataset. (LA-UR-20-22636)

Korobkin, O., W. P. Even and R. T. Wollaeger. Extended parameter cube of models from Even et al. (2019). Dataset. (LA-UR-19-30245)

Miller, J. M., J. Lippuner, R. T. Wollaeger, T. M. Sprouse and M. R. Mumpower. Simulations of Neutrino-Driven Accretion Flows. Dataset. (LA-UR-20-29317)

Mumpower, M. R. rapid neutron capture process videos. Audio/Visual. (LA-UR-21-23900)

Mumpower, M. R. and G. W. Misch. Nuclear cross sections on ground and excited states. Dataset. (LA-UR-21-29293)

Salvesen, G. M. and J. M. Miller. Black Hole Spin in X-ray Binaries: Giving Uncertainties an f. Dataset. (LA-UR-20-28697)

Ultra-Cold Neutron Experiment for Proton Branching Ratio in Neutron Beta Decay (UCNProBe)

Zhaowen Tang
20190048ER

Project Description

The free neutron decay lifetime is vital across many fields of physics. The Department of Energy Office of Science, Nuclear Physics has identified resolving the beam and bottle neutron lifetime discrepancy as a prerequisite to the next generation neutron lifetime experiments. The successful execution of this project will position the Laboratory to solve this lifetime discrepancy. The confirmation of the bottle lifetime results will be a vital piece of information for the nuclear physics community and help pave the way for a next generation ultracold neutron (UCN) based lifetime experiment; the confirmation of the beam lifetime results would demonstrate beyond the Standard Model (SM) of physics, and be truly extraordinary.

Publications

Journal Articles

*Tang, Z., E. B. Watkins, S. M. Clayton, S. A. Currie, D. E. Fellers, M. T. Hassan, D. E. Hooks, T. M. Ito, S. K. Lawrence, S. W. T. MacDonald, M. Makela, C. L. Morris, L. P. Neukirch, A. Saunders, C. M. O'Shaughnessy, C. Cude-Woods, J. H. Choi, A. R. Young, B. A. Zeck, F. Gonzalez, C. Y. Liu, N. C. Floyd, K. P. Hickerson, A. T. Holley, B. A. Johnson, J. C. Lambert and R. W. Pattie. Ultracold neutron properties of the Eljen-299-02D deuterated scintillator. 2021. *Review of Scientific Instruments*. **92** (2): 023305. (LA-UR-20-27508 DOI: 10.1063/5.0030972)

Presentation Slides

Hassan, M. T. An experiment to measure the Proton Branching Ratio in Neutron Beta Decay (UCNProBe). Presented at *APS DNP 2019*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30666)

Hassan, M. T. The current status of the UCNProBe experiment. Presented at *APS DNP 2021*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-30177)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *Particle Physics with Neutrons at the ESS*, stockholm, Sweden, 2018-12-10 - 2018-12-14. (LA-UR-18-31486)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *APS April Meeting 2019*, denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23299)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *Fundamental physics with neutron beta decay*, Seattle, Washington, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31233)

Tang, Z., C. Morris, J. H. Choi and D. E. Fellers. Search for the Neutron Decay n\xe2\x9f\xb6\xf0\x9d\x9b\xbe+X, where X is a dark matter particle. Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30026)

Tang, Z., J. C. Lambert, C. Morris and S. Clayton. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30027)

Tang, Z. and N. C. Floyd. Ultra-Cold Neutron measurement of the Proton branching ratio in neutron Beta Decay (UCNProBe). Presented at *APS DNP 2020*, Virtual, New Mexico, United States, 2020-10-29 - 2020-11-02. (LA-UR-20-28876)

Wideband Sub-Millimeter Source for Deployed Applications

Kip Bishofberger
20190066ER

Project Description

We are developing a wideband amplifier system that can yield significant power over a wide range of frequencies. The system is compact and power-efficient for low size, weight, and power applications. Project results could potentially impact several Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) mission areas. Several potential future applications are described below. Project results could impact Mono/bistatic Radar Time-domain Spectroscopy. Results from this project could ultimately support a capability to probe a cloud, smoke column, or atmospheric region. A large bandwidth would allow one system to be used to detect a wide variety of chemical signatures. Project results could impact Space-based Spectroscopy; future applications could allow most of the atmospheric column to be analyzed via a system deployed from orbit. Project results could impact Secure Communications; a small wavelength would enable small antennas to communicate (at very high bandwidths), without unintended listeners (e.g., satellites, aircraft, binoculars). Project results could impact Materials Inspection; although dielectrics are transparent, the high resolution anticipated through this project would ultimately allow the detection of millimeter-scale features (e.g., high-Z, circuitry) for improvised explosive device (IED) and special nuclear material (SNM detection).

Publications

Journal Articles

Yampolsky, N. and K. A. Bishofberger. Description of longitudinal space charge effects in beams and plasma through dielectric permittivity. Submitted to *Physical Review Applied*. (LA-UR-21-21464)

Conference Papers

Neben, D. E., K. A. Bishofberger, V. Pavlenko and N. Yampolsky. Design of a Source for Millimeter-wave Ultra-wide Bandwidth Applications Using the Two-stream Instability. Presented at *International Vacuum Electronics Conference*. (Monterey, California, United States, 2020-04-20 - 2020-04-23). (LA-UR-20-21994)

Presentation Slides

Neben, D. E. Ultra Wide Bandwidth Source Utilizing the Two Stream Instability. . (LA-UR-21-27587)

Posters

Neben, D. E., N. Yampolsky, K. A. Bishofberger and V. Pavlenko. Design of a Source for Millimeter-wave Ultra-wide Bandwidth Applications Using the Two-Stream Instability. Presented at *IVEC 2020*, Monterey, California, United States, 2020-10-17 - 2020-10-17. (LA-UR-20-27600)

Neben, D. E., N. Yampolsky, V. Pavlenko and K. A. Bishofberger. A TEST SOURCE FOR THE PRODUCTION OF MILLIMETER-WAVE RF USING THE TWO-STREAM INSTABILITY. Presented at *ICOPS 2020*, Los Alamos, New Mexico, United States, 2020-12-06 - 2020-12-06. (LA-UR-20-29912)

Ultralight Bosonic Dark Matter Search with an Optically Pumped Magnetometer

Leanne Duffy
20190113ER

Project Description

Modern cosmological observations lead to the conclusion that most of the matter in the Universe is of an undiscovered form. Matter that interacts with light contributes only 20% of the Universe's matter, with the remaining 80% given by dark matter, inferred via its gravitational effects on visible matter and radiation. Discovering the nature of dark matter is one priority of Cosmic Frontier research funded by the Department of Energy Office of Science, High Energy Physics program. Los Alamos National Laboratory has a unique intersection of leadership in axion physics with world-leading magnetic field detection capabilities through the development and application of optically pumped magnetometers, and an existing magnet that can be applied to develop the next level of sensitivity in axion searches. We estimate that our proposed experiment can probe axion specific axion masses with a sensitivity that is up to 4 orders of magnitude beyond the existing best limit. Our ultimate goal is to reveal the nature of the Universe's dark matter. At the very least, we will provide significant new limits on the properties of the dark matter.

Publications

Reports

Milton, S. V. Review of LDRD ER Project 20190113ER. Unpublished report. (LA-UR-21-20385)

Presentation Slides

Duffy, L. D. Axion search with the Axion Dark Matter eXperiment and other new idea(s). . (LA-UR-20-28374)

Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)

Kim, Y. J., P. Chu, I. M. Savukov, S. G. Newman, L. D. Duffy and A. V. Urbaitis. Dark Matter and Fundamental Physics Searches using Atomic Magnetometers. Presented at *CPAD Instrumentation Frontier Workshop 2019*, Madison, Wisconsin, United States, 2019-12-08 - 2019-12-10. (LA-UR-19-31996)

Hot Electron Beam Generation and Transport for Fast Ignition

Sasikumar Palaniyappan
20190124ER

Project Description

Inertial confinement fusion (ICF) is one of the grand challenges of this century due to its potential to provide an unlimited amount of clean energy. In laser-driven ICF, a high-energy nanosecond laser compresses a mixture of deuterium (D) and tritium (T) fuel inside a capsule to very high-density and temperature and initiates nuclear fusion reactions. Despite decades of research, laboratory fusion is still elusive. Electron fast ignition is a variant of ICF where the fuel is first compressed to high density using a long-pulse (nanosecond) laser and then ignited by a hot-electron beam generated from a short-pulse (picosecond) laser interaction with a gold cone tip, where the short pulse laser is usually brought into the assembled dense fuel via a re-entrant cone. The current cone-in-shell design suffers due to large electron beam divergence. This proposal will address the crippling deficiencies in electron fast ignition by generating a near-collimated hot-electron beam using near-critical plasmas and transport it effectively from the source to the dense fuel with the aid of resistive magnetic collimation.

Publications

Journal Articles

Bhattacharjee, C. and D. J. Stark. Gravitomagnetic vorticity generation in black hole accretion disks: a potential spatial constraint on plasma flow stability. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-28722)

*S. P. *. P. S. *. H. C. Li, F. *., P. K. Singh, S. Palaniyappan, F. -. Li and C. -. Huang. Particle resonances and trapping of direct laser acceleration in a laser-plasma channel. 2021. *Physical Review Accelerators and Beams*. **24** (4): 041301. (LA-UR-21-25156 DOI: 10.1103/PhysRevAccelBeams.24.041301)

Li, F., P. K. Singh, S. Palaniyappan and C. Huang. Parameterization of nonlinear particle resonances in direct laser acceleration. Submitted to *Physical Review Letters*. (LA-UR-20-22447)

Singh, P. K., F. Li, C. Huang, A. Moreau, R. Hollinger, S. A. Junghans, A. Favalli, C. Calvi, S. Wang, Y. Wang, H. Song, J. Rocca, R. E. Reinovsky and S. Palaniyappan. Multi-stage MeV electron acceleration from laser-driven nano-foils undergoing relativistic transparency. Submitted to *Nature Physics*. (LA-UR-21-20711)

Singh, P. K., F. Li, S. A. Junghans, A. Favalli, R. E. Reinovsky, C. Huang, S. Palaniyappan, A. Moreau, R. Hollinger, C. Calvi, S. Wang, Y. Wang and J. J. Rocca. Cascade acceleration of MeV electrons during intense femtosecond laser-nanometer foil transparency. Submitted to *Physical Review Letters*. (LA-UR-20-24689)

Reports

Schmitt, M. J., B. J. Albright and E. N. Loomis. Los Alamos LDRD Appraisal Final Report for 20190124ER. Unpublished report. (LA-UR-21-31901)

Presentation Slides

Huang, C., F. Li, P. K. Singh and S. Palaniyappan. Transport of low-divergence high-current electron beams in a high density plasma. Presented at *49th Annual Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-10 - 2019-06-14. (LA-UR-19-25186)

Li, F. Laser-plasma based electron acceleration and its applications. . (LA-UR-20-24276)

Li, F., C. Huang, P. K. Singh and S. Palaniyappan. Electron beam properties from combined direct laser acceleration and plasma acceleration in regimes relevant to fast ignition. Presented at *49th Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-14. (LA-UR-19-25253)

Li, F., C. Huang, P. K. Singh and S. Palaniyappan. Towards controlled laser acceleration of electrons in laser-plasma coupling regimes relevant to fast ignition. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30695)

Singh, P. K., F. Li, S. A. Junghans, C. Huang, A. Favalli, R. E. Reinovsky, S. Palaniyappan, A. Moreau, R. Hollinger, C. Calvi, S. Wang, Y. Wang, H. Song and J. J. Rocca. Cascade acceleration of MeV electrons during intense femtosecond laser-nanometer foil transparency. Presented at *62nd Annual Virtual Meeting of the APS Division of*

Effects of Strong Electronic Correlations on the Properties of Warm Dense Matter

Jerome Daligault
20200074ER

Project Description

The issues we address affect national energy and security missions at Los Alamos, which require high-fidelity computer simulations that rely on accurate plasma properties over a wide range of physical conditions, and in particular of warm dense matter (WDM) conditions that occur during the implosion phase of inertial confinement fusion capsules and in nuclear explosions. By its intermediate nature, the WDM regime does not fall neatly within the parameter space typical of either ordinary condensed-matter physics or plasma physics, and the standard simplifying approximations of these fields no longer apply. As a consequence, our theoretical understanding of this extreme state of matter relies mostly on advanced computer simulations. The new computational tool we will develop in this project will significantly advance our predicting capability of properties of WDM. This will be a new, world-class capability to model extreme states of matter at the Laboratory that will support both discovery research and programmatic applications at the forefront of an exciting and rapidly growing field. We will apply our much-improved electronic structure calculations to several pressing questions in support of current and future experiments.

Publications

Journal Articles

*Bernstein, D. J., T. Lafleur, J. Daligault and S. D. Baalrud. Friction force in strongly magnetized plasmas. 2020. *Physical Review E*. **102** (4): 041201. (LA-UR-20-23660 DOI: 10.1103/PhysRevE.102.041201)

Bernstein, D. J., T. Lafleur, J. O. Daligault and S. D. Baalrud. Friction Force in Strongly Magnetized Plasmas. Submitted to *Physical Review E*. (LA-UR-20-25004)

Daligault, J. O., J. Simoni, Q. L. Nguyen, K. M. Dorney, J. L. Ellis, N. J. Brooks, D. D. Hickstein, A. N. Grennell, X. Shi, S. Yazdi, E. E. Campbell, H. C. Kapteyn and M. M. Murnane. Mapping the electron-phonon coupling and hot electron cooling in copper nanoparticles in the warm-dense regime. Submitted to *Nature Physics*. (LA-UR-20-24971)

Daligault, J. O. and J. Simoni. Electronic Friction in Warm Dense Matter. Submitted to *Physical Review Letters*. (LA-UR-20-22846)

Daligault, J. O. and J. Simoni. Effects of temperature on the spectrum of single-particle excitations in the homogeneous electron gas. Submitted to *Physical Review B*. (LA-UR-21-28725)

*Simoni, J. and J. Daligault. Nature of Non-Adiabatic Electron–Ion Forces in Liquid Metals. 2020. *The Journal of Physical Chemistry Letters*. **11** (20): 8839-8843. (LA-UR-20-25020 DOI: 10.1021/acs.jpclett.0c02134)

*Stolyarov, E. V., A. J. White and D. Mozyrsky. Mixed quantum–classical approach to model non-adiabatic electron–nuclear dynamics: Detailed balance and improved surface hopping method. 2020. *The Journal of Chemical Physics*. **153** (7): 074116. (LA-UR-20-24033 DOI: 10.1063/5.0014284)

Exploration of Neutron-Star Crust Dynamics in the Era of Gravitational-Wave Astrophysics

Irina Sagert
20200145ER

Project Description

This project will quantify of the role of the solid neutron-star crust in neutron-star mergers. Dynamical studies of mergers with realistic microphysical input have only recently become feasible. We will be the first ones to include the solid crust. Neutron-star material is too dense and neutron-rich to be attained in laboratories and its study complements experiments as done by e.g. the Facility for Rare Isotope Beams. In our work, we will disentangle its effect from the nuclear equation of state in gravitational wave and electromagnetic signatures of merger events. Our results will be crucial for gravitational wave detectors like the Laser Interferometer Gravitational-wave Observatory (LIGO) and Virgo, and be important for gamma-ray observatories as the National Aeronautics Space Administration's Fermi and Chandra missions. This work will use state-of-the-art nuclear physics input to answer fundamental questions about the states of matter following the Department of Energy's Long Range Plan of Nuclear Science. We will deliver complex multi-physics codes that scale to the largest machines available and apply these codes in the to the most extreme conditions that exist in the universe. This will benefit the Advanced Scientific Computing Program by providing insights into improving simulation capability, reliability, and scalability.

Publications

Journal Articles

*W. R. T. *. F. C. L. *. H. A. L. *. R. S. *. F. C. J. *. M. M. R. *. C. E. A. *. E. W. P. *. M. J. *. M. G. W. *. L. J. Korobkin, O. *., O. Korobkin, R. T. Wollaeger, C. L. Fryer, A. L. Hungerford, C. J. Fontes, M. R. Mumpower, E. A. Chase, W. P. Even, G. W. Misch, J. Lippuner and J. Miller. Axisymmetric Radiative Transfer Models of Kilonovae. 2021. *The Astrophysical Journal*. **910** (2): 116. (LA-UR-20-22607 DOI: 10.3847/1538-4357/abe1b5)

*Loiseau, J., H. Lim, M. A. Kaltenborn, O. Korobkin, C. M. Mauney, I. Sagert, W. P. Even and B. K. Bergen. FleCSPH: The next generation FleCSIble parallel computational infrastructure for smoothed particle hydrodynamics. 2020. *SoftwareX*. **12**: 100602. (LA-UR-20-23626 DOI: 10.1016/j.softx.2020.100602)

*Murakami, M., O. Korobkin and G. Zhang. Time-dependent density-functional theory of high-order harmonic generation from noble-gas atoms driven by orthogonally polarized two-color laser fields. 2020. *Physical Review A*. **101** (6): 063413. (LA-UR-20-22847 DOI: 10.1103/PhysRevA.101.063413)

Tsao, B., R. Haas and A. Tsokaros. Source term method for binary neutron stars initial data. Submitted to *Journal of Computational Physics*. (LA-UR-20-28227)

Conference Papers

Korobkin, O., H. Lim, J. Loiseau, C. M. Mauney, I. Sagert, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *Spheric 2021*. (Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11). (LA-UR-21-24198)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *Spheric 2021*. (Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11). (LA-UR-21-24191)

Reports

Korobkin, O. Institutional Computing 2019/2020 Project Report: First Year. Unpublished report. (LA-UR-20-25524)

Korobkin, O. Institutional Computing 2019/2020 Allocation Report: Viewgraphs, Year 1. Unpublished report. (LA-UR-20-25615)

Lim, H. FleCSPH Wiki. Unpublished report. (LA-UR-20-26581)

Presentation Slides

Korobkin, O. Mergers of Compact Objects with SPH and General Relativity, Allocation: w20_nsmergers (year 1). . (LA-UR-21-22056)

Lim, H. Are we alone? Searching Intelligent Life Beyond the Earth. . (LA-UR-20-25542)

Lim, H. Enhancing FleCSPH Features and Validation Tests. . (LA-UR-22-21572)

Lim, H., O. Korobkin, J. Loiseau, C. M. Mauney, I. Sagert, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *Spheric 2021*, Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25052)

Lim, H., O. Korobkin, J. Loiseau, C. M. Mauney, I. Sagert, M. A. R. Kaltenborn, B. Tsao and W. P. Even. Conservation of Angular Momentum in the Fast Multipole Method. Presented at *Spheric 2021*, Virtually Anywhere, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25190)

Lo, L., A. R. Stewart, O. Korobkin and J. Loiseau. Visualization of a Neutron Star Binary Merger and Subsequent Creation of Kilonova. Presented at *Supercomputing Conference 2021*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14. (LA-UR-21-27889)

Sagert, I. Exploring Nuclear Astro-Materials in Neutron Stars with Numerical Simulations. Presented at *Computing Research Leadership Council Virtual Series*, Virtual, New Mexico, United States, 2021-04-16 - 2021-04-16. (LA-UR-21-23630)

Sagert, I., O. Korobkin, B. Tsao, I. Tews, H. Lim and J. Loiseau. Modeling Astrophysical Solids with FleCSPH. Presented at *APS April Meeting*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-23237)

Sagert, I., O. Korobkin, B. Tsao and H. Lim. Studying Crust-Breaking Events in Neutron Stars with Strength and Smoothed Particle Hydrodynamics. . (LA-UR-21-21876)

Sagert, I., O. Korobkin, M. A. R. Kaltenborn, H. Lim, J. Loiseau, C. M. Mauney, I. Tews, B. Tsao and W. P. Even. Overview of FleCSPH Solid Material Modeling Capabilities. . (LA-UR-21-25175)

Sagert, I. and O. Korobkin. Studying Crust-Breaking Events in Neutron Stars with Strength and Smoothed Particle Hydrodynamics. . (LA-UR-20-21887)

Stewart, A. R., L. Lo, O. Korobkin, I. Sagert, J. Loiseau, H. Lim, M. A. R. Kaltenborn, C. M. Mauney and J. M. Miller. Visualization of a Neutron Star Binary Merger and Subsequent Creation of Kilonova. Presented at *Supercomputing 2021*, St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14. (LA-UR-21-28564)

Tews, I. Stringent constraints on neutron-star radii from neutron-star mergers and chiral effective field theory. Presented at *Hirschegg 2020*, Hirschegg, Austria, 2020-01-13 - 2020-01-13. (LA-UR-20-20236)

Tsao, B. Smooth Particle Hydrodynamics for Neutron Star Oscillation with General Relativistic effects. Presented at *LANL Astrophysics seminar*, Los Alamos, New Mexico, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-22758)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *SPHERIC 2021*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25313)

Tsao, B., I. Sagert, O. Korobkin, I. Tews, H. Lim, G. A. Dilts and J. Loiseau. Modeling Neutron Star Oscillations in a Fixed General Relativistic Background Including Solid Crust Dynamics. Presented at *SPHERIC 2021*, Los Alamos, New Mexico, United States, 2021-06-07 - 2021-06-11. (LA-UR-21-25319)

Posters

Lim, H., O. Korobkin, J. M. Miller, R. T. Wollaeger, C. J. Fontes, M. A. R. Kaltenborn, W. P. Even and J. Loiseau. Studying Expansion of Ejecta from Binary Neutron Star Mergers. Presented at *Aps April Meeting 2021*, Virtually Anywhere, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23238)

Tsao, B., O. Korobkin, H. Lim, I. Sagert, I. Tews and J. Loiseau. Studying Neutron Star Oscillations with General Relativistic Smoothed Particle Hydrodynamics. Presented at *APS April meeting 2021*, virtual, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23327)

Other

Lim, H. Are we alone? Searching Intelligent life beyond the Earth. Audio/Visual. (LA-UR-20-27695)

Novel X-ray Free-electron Lasers (XFEL) Accelerator Architecture

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Project Description

X-ray free-electron lasers (XFELs) are billion-dollar-class scientific instruments used for discovery science in materials, biology, and chemistry, and also for national security applications. For example, Los Alamos has identified an XFEL as a potential tool to address developing a needed future capability for ensuring the viability of the nation's nuclear assets, the dynamic mesoscale materials science capability (DMMSC). Despite their cost, the broad impact of XFELs has led to the recent development of a half-dozen XFEL facilities worldwide, including one already operating in the United States and another coming on-line in a few years. Their high cost results from electron beam instabilities in the accelerators driving the XFELs, which presently can only be mitigated by increasing the electron beam energy. This in turn requires a longer (and more expensive) accelerator. The goal of this project is to investigate if a novel accelerator architecture generating a microbunched electron beam can suppress these instabilities to the point that significantly lower electron beam energies (and thus a much less expensive accelerator) can be used to drive XFELs. If so, this approach may lead to XFELs inexpensive enough that they can become university-laboratory sized tools.

Publications

Journal Articles

*Rosenzweig, J. B., N. Majernik, R. R. Robles, G. Andonian, O. Camacho, A. Fukasawa, A. Kogar, G. Lawler, J. Miao, P. Musumeci, B. Naranjo, Y. Sakai, R. Candler, B. Pound, C. Pellegrini, C. Emma, A. Halavanau, J. Hastings, Z. Li, M. Nasr, S. Tantawi, P. Anisimov, B. Carlsten, F. Krawczyk, E. Simakov, L. Faillace, M. Ferrario, B. Spataro, S. Karkare, J. Maxson, Y. Ma, J. Wurtele, A. Murokh, A. Zholents, A. Cianchi, D. Cocco and S. B. van der Geer. An ultra-compact x-ray free-electron laser. 2020. *New Journal of Physics*. **22** (9): 93067. (LA-UR-20-29584 DOI: 10.1088/1367-2630/abb16c)

Presentation Slides

Anisimov, P. M., D. C. Nguyen and N. Neveu. Time-independent 3D FEL Simulations. . (LA-UR-21-20607)

Anisimov, P. M., D. C. Nguyen and N. Neveu. Time-dependent 3D FEL Simulations. . (LA-UR-21-20803)

Anisimov, P. M., N. Neveu and D. C. Nguyen. Introduction to FEL Simulations. . (LA-UR-21-20608)

Carlsten, B. E. Accelerator technology studies for X-ray FELs. . (LA-UR-21-27087)

Neveu, N., P. M. Anisimov and D. C. Nguyen. Optimization and Beam Shaping. . (LA-UR-21-21188)

Nguyen, D. C., P. M. Anisimov, Y. Li and N. Neveu. Self-Seeding, Regenerative Amplifier FEL & XFELO. . (LA-UR-21-21184)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Introduction, Electron Motions in an Undulator, Undulator Radiation & FEL. . (LA-UR-21-20610)

Nguyen, D. C., P. M. Anisimov and N. Neveu. SASE, High-Gain FEL & 1D Theory. . (LA-UR-21-20609)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Harmonic Generation, HGHG & EEHG. . (LA-UR-21-21185)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Electron Bunch Compression, CSR, mBi, Laser Heater & Machine Layout. . (LA-UR-21-21190)

Nguyen, D. C., P. M. Anisimov and N. Neveu. Photoinjectors, Emittance Revisited, Photoinjector Design & Optimization. . (LA-UR-21-21187)

MixIT – Understanding Mix in Fusion Implosions through Ion Temperature Imaging

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Project Description

This project will produce the first-ever spatially resolved ion temperature measurement of inertial confinement fusion (ICF) implosions. The novel measurement has the potential to uncover the missing piece on the path to ignition for future fusion facilities. Leveraging our expertise as world leaders in fusion neutron imaging we will enhance cutting-edge technology to determine plasma ion temperature – adding a transformational diagnostic capability to Los Alamos National Laboratory's toolkit for fusion research. The injection of contaminant mass into fuel regions - or mix - is believed to be a primary factor preventing ignition at the National Ignition Facility - the world's most powerful ICF facility. Knowledge of the temperature distribution in the hot spot will be crucial for determining accurate estimates of the amount of contaminant and for providing constraints on radiation-hydrodynamics modeling of ICF experiments. A better understanding of ICF burn and hydrodynamic mix does not only advance the United States fusion program, it also ties directly into our core mission of stockpile stewardship.

Publications

Presentation Slides

Birge, N. W., V. Geppert-Kleinrath, C. R. Danly, B. M. Haines, H. J. Jorgenson, E. F. Mendoza, L. R. Tafoya, P. L. Volegov and C. H. Wilde. MixIT: designing a 1D ion temperature imager for ICF. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30939)

Birge, N. W., V. Geppert-Kleinrath, C. R. Danly, P. L. Volegov, C. H. Wilde and B. M. Haines. Photometrics for the MixIT Project. . (LA-UR-20-27133)

Birge, N. W. and V. Geppert-Kleinrath. MixIT LDRD Lens Design. . (LA-UR-20-24227)

Geppert-Kleinrath, V. The Quest for Symmetry:\xc2\xa03D Nuclear Imaging of Inertial Confinement Fusion \xc2\xa0Implosions. Presented at *Laboratory for Laser Energetics, University of Rochester Seminar*, Rochester, New York, United States, 2021-12-10 - 2021-12-10. (LA-UR-21-32155)

Geppert-Kleinrath, V., P. L. Volegov, C. R. Danly, N. W. Birge, C. H. Wilde and B. M. Haines. MixIT – Understanding Mix in Fusion Implosions through Ion Temperature Imaging. Presented at *Physics Cafe*, Los Alamos, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-23206)

Mendoza, E. F., V. Geppert-Kleinrath, N. W. Birge and C. R. Danly. MCNP Simulations for Aperture Alignment In ICF Imaging. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27640)

The Missing Link: Quantum Mechanics in Plasma Kinetic Modeling

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Project Description

The tokamak disruption problem poses a serious threat to the future success of the International Thermonuclear Experimental Reactor (ITER), efficiently harnessing magnetic confinement nuclear fusion energy, and understanding energy production in civilian applications. During this project we will develop the Los Alamos atomic physics suite of codes to support the plasma modeling effort to design a tokamak disruption mitigation system. Los Alamos is the ideal venue for such research, as this problem requires a cross-disciplinary synergistic approach between atomic physicists, and plasma physicists, as well as the utilization of abundant computing resources and sophisticated atomic physics tools that are only available at Los Alamos. This project will contribute to the design and implementation of a disruption mitigation system that is required in the operations of ITER and future fusion tokamak facilities. The developments made during this project will have a direct application to inertial confinement fusion experiments.

Publications

Journal Articles

*Garland, N. A., H. Chung, C. J. Fontes, M. C. Zammit, J. Colgan, T. Elder, C. J. McDevitt, T. M. Wildey and X. Tang. Impact of a minority relativistic electron tail interacting with a thermal plasma containing high-atomic-number impurities. 2020. *Physics of Plasmas*. **27** (4): 040702. (LA-UR-19-28749 DOI: 10.1063/5.0003638)

Garland, N. A., H. K. Chung, M. C. Zammit, J. P. Colgan, C. J. Fontes and X. Tang. Understanding how minority relativistic electron populations may dominate charge state balance and radiative cooling of a post-thermal quench tokamak plasma. Submitted to *Physics of Plasmas*. (LA-UR-21-29190)

Garland, N. A., H. K. Chung, M. C. Zammit, J. P. Colgan, C. J. Fontes and X. Tang. Understanding how minority relativistic electron populations may dominate charge state balance and radiative cooling of a post-thermal quench tokamak plasma. Submitted to *Physics of Plasmas*. (LA-UR-21-29190)

Garland, N. A., R. Maulik, Q. Tang, X. Tang and P. Balaprakash. Efficient data acquisition and training of collisional-radiative model artificial neural network surrogates through adaptive parameter space sampling. Submitted to *Machine Learning: Science and Technology*. (LA-UR-21-31682)

Horton, R. K., D. V. Fursa, L. H. Scarlett, I. Bray and M. C. Zammit. Electron energy deposition in molecular hydrogen gas: a Monte-Carlo simulation using convergent close-coupling cross sections. Submitted to *Plasma Sources Science and Technology*. (LA-UR-21-26392)

Mori, N. A., R. Utamuratov, D. V. Fursa, M. C. Zammit and I. Bray. Calculation of the single differential cross section for electron-impact ionization of atoms and molecules. Submitted to *Physical Review A*. (LA-UR-20-23099)

Padovani, M., S. Bialy, D. Galli, A. Ivlev, T. Grassi, L. H. Scarlett, U. Rehill, M. C. Zammit, D. V. Fursa and I. Bray. Cosmic rays in molecular clouds probed by H2 rovibrational lines Perspectives for the James Webb Space Telescope. Submitted to *Astronomy and Astrophysics*. (LA-UR-21-29186)

Park, R. M., W. R. Kupets, M. C. Zammit, J. P. Colgan, C. J. Fontes, B. S. Scheiner, E. M. E. Timmermans, X. Tang, L. H. Scarlett, D. V. Fursa, I. Bray and N. A. Garland. Anisotropic angular scattering models of elastic electron-neutral collisions for Monte Carlo plasma simulations. Submitted to *Plasma Sources Science & Technology*. (LA-UR-21-32313)

Scarlett, L. H., D. K. Boyle, M. C. Zammit, Y. Ralchenko, I. Bray and D. V. Fursa. Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues: III. Vibrational excitation via electronic excitation and radiative decay.. Submitted to *Atomic Data and Nuclear Data Tables*. (LA-UR-22-22070)

Scarlett, L. H., D. V. Fursa, J. Knol, M. C. Zammit and I. Bray. Isotopic and vibrational-level dependence of H2 dissociation by electron impact. Submitted to *Physical Review A*. (LA-UR-20-29938)

Scarlett, L. H., J. S. Savage, D. V. Fursa, I. Bray, M. C. Zammit and B. I. Schneider. Convergent close-coupling calculations of electrons scattering on electronically-excited

molecular hydrogen. Submitted to *Physical Review A*. (LA-UR-20-30414)

Scarlett, L. H., U. S. Rehill, M. C. Zammit, D. V. Fursa, K. Bartschat and I. Bray. Calculated linear polarization fractions of Fulcher-\xce\xb1 fluorescence in electron collisions with H2. Submitted to *Physical Review A*. (LA-UR-21-27474)

Wu\xcc\x88nderlich, D., L. H. Scarlett, S. Briefi, U. Fantz, M. C. Zammit, D. V. Fursa and I. Bray. Application of Molecular Convergent Close-Coupling cross sections in a Collisional Radiative model for the triplet system of molecular hydrogen. Submitted to *Journal of Physics D: Applied Physics*. (LA-UR-20-27482)

Conference Papers

Garland, N. A., R. Maulik, Q. Tang, X. Tang and P. Balaprakash. Progress towards high fidelity collisional-radiative model surrogates for rapid in-situ evaluation. Presented at *Machine Learning and the Physical Sciences Workshop at the 34th Conference on Neural Information Processing Systems (NeurIPS)*. (Virtual (originally Vancouver), Canada, 2020-12-11 - 2020-12-11). (LA-UR-20-28192)

Reports

George, A., M. C. Zammit and N. A. Garland. Summer 2020 Los Alamos National Laboratory Report. Unpublished report. (LA-UR-21-24169)

George, A., M. C. Zammit and N. A. Garland. Summer 2020 Los Alamos National Laboratory Report. Unpublished report. (LA-UR-21-24169)

Presentation Slides

Colgan, J. P., M. C. Zammit, N. A. Garland, C. J. Fontes, X. Tang and M. Pindzola. Differential cross sections for the electron-impact ionization of neon. Presented at *DAMOP 2021*, Virtual, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25163)

Colgan, J. P., M. C. Zammit, N. A. Garland, J. Li, C. J. Fontes, X. Tang and M. S. Pindzola. Angular distributions for electron-impact ionization of noble gases and their application to plasma modeling. Presented at *DAMOP 2020*, Portland, Oregon, United States, 2020-06-02 - 2020-06-02. (LA-UR-20-24064)

Garland, N. A. Impact of a minority relativistic electron tail interacting with a thermal plasma containing high-atomic-number impurities. . (LA-UR-20-23791)

Garland, N. A., A. George and M. C. Zammit. Uncertainty quantification of atomic data for collisional-radiative modeling of fusion plasmas. Presented at *LANL T-Div Student Lightning talks*, Los Alamos, New Mexico, United States, 2020-08-04 - 2020-08-04. (LA-UR-20-25815)

Garland, N. A., M. C. Zammit, C. J. Fontes, J. P. Colgan, H. K. Chung and X. Tang. A collisional-radiative model

benchmarking and comparative study of fusion relevant atoms. Presented at *GEC 2020*, San Diego, California, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-28191)

George, A., N. A. Garland and M. C. Zammit. Collisional Radiative model for nuclear fusion. . (LA-UR-20-24941)

George, A., W. R. Kupets, N. A. Garland and M. C. Zammit. Uncertainty quantification of atomic data for collisional-radiative modeling of fusion plasmas. . (LA-UR-21-24165)

George, A., W. R. Kupets, N. A. Garland and M. C. Zammit. Uncertainty quantification of atomic data for collisional-radiative modeling of fusion plasmas. . (LA-UR-21-24165)

Kupets, W. R., N. A. Garland, J. P. Colgan, C. J. Fontes, X. Tang, I. Bray, D. V. Fursa, L. H. Scarlett and M. C. Zammit. Comparisons and fits of electron angular distribution approximations for elastic scattering from neutral fusion-relevant targets. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Virtual Conference, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25045)

Kupets, W. R., N. A. Garland, J. P. Colgan, C. J. Fontes, X. Tang, I. Bray, D. V. Fursa, L. H. Scarlett and M. C. Zammit. Comparisons and fits of electron angular distribution approximations for elastic scattering from neutral fusion-relevant targets. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Virtual Conference, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25045)

Park, R. M., M. C. Zammit, W. R. Kupets, J. P. Colgan, C. J. Fontes, X. Tang, L. H. Scarlett, D. V. Fursa, I. Bray and N. A. Garland. LOW-TEMPERATURE PLASMA TRANSPORT COEFFICIENTS DERIVED FROM SCATTERING ANGULAR DISTRIBUTION FUNCTIONS. . (LA-UR-21-27525)

Zammit, M. C., J. A. Leiding, J. C. A. O. Jung, J. P. Colgan, C. J. Fontes, D. P. Kilcrease, P. Hakel, E. M. E. Timmermans, D. V. Fursa and I. Bray. First-Principles Molecular Spectra for Air and Astrophysical Plasmas. Presented at *73rd Annual Gaseous Electronics Virtual Conference*, San Diego, California, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-27919)

Zammit, M. C., J. P. Colgan, D. P. Kilcrease, C. J. Fontes, P. Hakel, J. A. Leiding, J. C. A. O. Jung, E. M. E. Timmermans, J. S. Savage, D. V. Fursa, A. S. Kadyrov, I. Bray, M. Charlton, S. Jonsell and R. C. Forrey. Molecular Data for Atmospheric Physics, Plasma Modeling and Antimatter Molecule Production. Presented at *GEM XXI ATMOP 2020*, Canberra, Australia, 2020-02-11 - 2020-02-11. (LA-UR-20-21966)

Zammit, M. C., J. P. Colgan, D. P. Kilcrease, C. J. Fontes, P. Hakel, J. A. Leiding, J. C. A. O. Jung, E. M. E. Timmermans, J. S. Savage, D. V. Fursa, A. S. Kadyrov, I. Bray, M. Charlton, S. Jonsell and R. C. Forrey. Molecular Data for Atmospheric Physics, Plasma Modeling and Antimatter Molecule Production. . (LA-UR-20-22047)

Zammit, M. C., N. A. Garland, W. R. Kupets, J. P. Colgan, C. J. Fontes, J. Li and X. Tang. FY20 Appraisal: The Missing Link? Quantum Mechanics in Plasma Kinetic Modeling. . (LA-UR-20-29400)

Zammit, M. C., N. A. Garland, W. R. Kupets, R. M. Park, J. P. Colgan, C. J. Fontes and X. Tang. FY21 Appraisal: The Missing Link? Quantum Mechanics in Plasma Kinetic Modeling. . (LA-UR-22-20060)

How do Pulsar Winds Shine in Tera Electron Volt (TeV)?

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Project Description

This project aims at understanding the origin of multi-Tera Electron Volt (TeV) emission from pulsar wind nebulae powered by termination shocks created by relativistic pulsar winds. This is a fundamental question in our understanding of the cosmos. This project brings together theory, numerical modeling, and multi-wavelength observations including gamma-rays. It builds capabilities in particle and gamma-ray detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Publications

Journal Articles

Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. Dahlin, Q. Zhang, J. Karpen and C. R. Devore. Slow Shock Formation Upstream of Reconnecting Current Sheets. Submitted to *Astrophysical Journal*. (LA-UR-21-27254)

Chen, Q., K. Nalewajko and B. P. Mishra. Scaling of Magnetic Dissipation and Particle Acceleration in ABC Fields. Submitted to *Journal of Plasma Physics*. (LA-UR-21-20632)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

Guo, F., X. Li, W. S. Daughton, H. Li, P. F. H. Kilian, Y. H. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics and Particle Acceleration during Relativistic Turbulent Magnetic Reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-26005)

*Guo, F., Y. Liu, X. Li, H. Li, W. Daughton and P. Kilian. Recent progress on particle acceleration and reconnection physics during magnetic reconnection in the magnetically-dominated relativistic regime. 2020. *Physics of Plasmas*. **27** (8): 080501. (LA-UR-20-26135 DOI: 10.1063/5.0012094)

Harding, A. K., C. Kalapotharakos, D. Kzanas and Z. Wadiasingh. The Multipolar Magnetic Field of the Millisecond Pulsar PSR J0030+0451. 2021. *The Astrophysical Journal*. **907** (2): 63. (LA-UR-21-22815 DOI: 10.3847/1538-4357/abcec0)

Harding, A. K. and C. Venter. Very-High-Energy Emission From Pulsars. Submitted to *Astrophysical Journal*. (LA-UR-21-30389)

*Harding, A. K. and G. Younes. Broadband X-ray burst spectroscopy of the fast-radio-burst-emitting Galactic magnetar. 2021. *Nature Astronomy*. **5** (4): 408-413. (LA-UR-21-22817 DOI: 10.1038/s41550-020-01292-x)

Harry, A., J. Drake, M. Swisdak, F. Guo, J. Dahlin, B. Chen, G. Fleishman, L. Glesener, K. Eduard, T. Phan and C. Shen. Electron Acceleration during Macroscale Non-Relativistic Magnetic Reconnection. Submitted to *Physical Review Letters*. (LA-UR-20-30073)

*Kilian, P., X. Li, F. Guo and H. Li. Exploring the Acceleration Mechanisms for Particle Injection and Power-law Formation during Transrelativistic Magnetic Reconnection. 2020. *The Astrophysical Journal*. **899** (2): 151. (LA-UR-20-20135 DOI: 10.3847/1538-4357/aba1e9)

Kong, X., F. Guo, C. Shen, B. Chen, Y. Chen and J. Giacalone. Dynamical modulation of solar flare electron acceleration due to plasmoid-shock interactions in the looptop region. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-30072)

Lazarian, A., O. Khabarova, S. Xu and F. Guo. Violation of Flux Freezing, Turbulent Magnetic Reconnection and induced Particle Acceleration. Submitted to *Review of Modern Plasma Physics*. (LA-UR-21-27253)

Li, X., F. Guo and Y. Liu. The Acceleration of Charged Particles and Formation of Power-law Energy Spectra in Nonrelativistic Magnetic Reconnection. Submitted to *Physics of Plasmas*. (LA-UR-21-21365)

Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. *PoS - Proceedings of Science*. (LA-UR-21-25495 DOI: 10.22323/1.395.0810)

Malone, K. A. A search for spectral hardening in HAWC sources above 56 TeV. *PoS - Proceedings of Science*. (LA-UR-21-25494 DOI: 10.22323/1.395.0811)

Malone, K. A., J. P. Harding, B. L. Dingus, M. Durocher, A. Albert, H. Zhou, C. Brisbois and V. Baghmanyan. Evidence that Ultra-High-Energy Gamma Rays are a Universal Feature Near Powerful Puslars. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-20344)

Mori, K., H. An, K. A. Malone, C. Hailey, B. Humensky, B. L. Dingus, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR broad-band X-ray observational campaign of energetic pulsar wind nebulae in synergy with VERITAS, HAWC and Fermi gamma-ray telescopes. *PoS - Proceedings of Science*. (LA-UR-21-26689 DOI: 10.22323/1.395.0963)

Pongkitiwanichakul, P., D. Ruffolo, F. Guo, S. Du, P. Suetrong, C. Yannawa, K. Makwana and K. Malakit. Role of Parallel Component of Solenoidal Electric Field on Conversion of Magnetic Energy into Plasma Kinetic Energy in 2D Decaying Turbulence. Submitted to *Astrophysical Journal*. (LA-UR-21-27251)

Yu, F., X. Kong, F. Guo, Y. Chen and J. Giacalone. Double-power-law feature in the energy spectra of energetic particles accelerated at coronal shocks. Submitted to *Astrophysical Journal*. (LA-UR-21-27255)

Zhang, H., X. Li, D. Giannios, F. Guo, H. Thiersen, M. Bottcher, T. Lewis and T. Venters. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–II. Connection with gamma-rays. Submitted to *Astrophysical Journal*. (LA-UR-21-27252)

Zhang, H., X. Li, D. Giannios, F. Guo, Y. H. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–I. A. Submitted to *Astrophysical Journal*. (LA-UR-20-27998)

Zhang, Q., F. Guo, W. S. Daughton, X. Li and H. Li. Efficient Nonthermal Ion and Electron Acceleration Enabled by the Flux-Rope KinkInstability in 3D Nonrelativistic Magnetic Reconnection. Submitted to *Physical Review Letters*. (LA-UR-21-24459)

zhang, h., X. Li, F. Guo and D. Giannios. First-Principle Prediction of X-ray Polarization from Magnetic Reconnection in High-Frequency BL Lacs. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-30074)

Presentation Slides

Durocher, M. TeV astrophysics with the HAWC observatory. Presented at *APS Four Corners Virtual Meeting*, Albuquerque, New Mexico, United States, 2020-10-23 - 2020-10-24. (LA-UR-20-28463)

Durocher, M. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *APS April 2021*, Washington, District Of Columbia, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23269)

Durocher, M. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30472)

Durocher, M. Limits on Diffuse Dark Matter with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30475)

Durocher, M. Searching for the Diffuse Gamma-Ray Background with HAWC. . (LA-UR-21-30456)

Durocher, M. Searching for the Diffuse Gamma-Ray Background with HAWC. Presented at *APS Four Corners Virtual Meeting 2021*, Boulder, Colorado, United States, 2021-10-08 - 2021-10-09. (LA-UR-21-30454)

Durocher, M. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30450)

Durocher, M. Limits on Diffuse Dark Matter with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30451)

Durocher, M. Finding a gamma ray in a haystack. . (LA-UR-21-30455)

Durocher, M. TeV Astrophysics with the HAWC Observatory. Presented at *37th Annual New Mexico Symposium*, Albuquerque, New Mexico, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31919)

Guo, F. Determining the Dominant Acceleration Mechanism during Relativistic Magnetic Reconnection in Large-scale Systems. Presented at *seminar in University of Tokyo.*, Tokyo, Japan, 2020-03-09 - 2020-03-13. (LA-UR-20-20430)

Guo, F. First Principles Kinetic Simulations of Relativistic Collisionless Shocks and Their Particle Acceleration (2019). . (LA-UR-20-25827)

Guo, F. First Principles Kinetic Simulations of Relativistic Collisionless Shocks and Their Particle Acceleration. . (LA-UR-20-25828)

Guo, F. Particle Acceleration in Magnetic Reconnection: From Small Scale to Large Scale. Presented at *2020 Magnetic Reconnection Workshop*, Weihai, China, 2020-08-24 - 2020-08-25. (LA-UR-20-26501)

Harding, J. P. and M. Durocher. Limits on the Diffuse Gamma-Ray Background with HAWC. Presented at *Virtual APS April Meeting*, Washington, District Of Columbia, United States, 2020-04-18 - 2020-04-18. (LA-UR-20-22988)

H. Kilian, P. F. Numerical Plasma Physics. . (LA-UR-20-23604)

H. Kilian, P. F., X. Li, F. Guo and H. Li. How magnetic reconnection injects particles and accelerates them to high energies. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-22043)

H. Kilian, P. F., X. Li, F. Guo and H. Li. Exploring the acceleration mechanisms for particle injection and power-law formation during trans-relativistic magnetic reconnection. Presented at *Understanding the Most Energetic Cosmic Accelerators: Advances in Theory and Simulation*, Online, New Mexico, United States, 2020-10-28 - 2020-10-30. (LA-UR-20-28623)

H. Kilian, P. F. and F. Guo. Particle Acceleration due to Relativistic Reconnection. Presented at *235th AAS meeting*, Honolulu, Hawaii, United States, 2020-01-05 - 2020-01-08. (LA-UR-20-20084)

Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25532)

Malone, K. A. HAWC results on other TeV halos. Presented at *1st Workshop on Gamma-ray Halos around Pulsars*, Rome (Virtual), Italy, 2020-12-01 - 2020-12-03. (LA-UR-20-29726)

Malone, K. A. HAWC study of the ultra-high-energy gamma-ray source MGRO J1908+06. Presented at *APS April 2021*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-23172)

Malone, K. A., K. Mori, B. L. Dingus, H. An, C. J. Hailey, B. Humensky, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR X-ray observation campaign of energetic pulsar wind nebulae. Presented at *International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-26302)

Posters

Durocher, M. Limits on Diffuse Dark Matter with HAWC. Presented at *37th International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-30453)

Malone, K. A. A search for spectral hardening in HAWC sources above 56 TeV. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25493)

A Dynamical Approach to Low-Energy Fission

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Project Description

Fission yields are important for a variety of applications and for our basic scientific understanding of the fission process and many-body nuclear physics. For nonproliferation purposes, fission fragments represent the initial conditions that decide upon the emission of neutron and gamma emission, which constitute signatures of specific nuclear materials. For nuclear forensics, fission yields are needed to identify the fuel and determine the neutron spectra that can be used to reconstruct and infer specific designs. For stockpile stewardship, fission yields are also needed to interpret historical data. For nuclear energy and nuclear waste management purposes, fission yields are needed in a large range of applications, like decay heat, shielding, dosimetry, fuel handling and safe waste disposal. They are also critical to properly perform a fission product inventory at each stage of the nuclear fuel cycle in reactors. Other applications include safeguards for nuclear reactor monitoring and medical applications for radioisotope production. This work is directed at improving the modeling capabilities needed in such applications, by implementing state-of-the art theoretical models capable of producing fission yields to be used in a variety of applications.

Publications

Journal Articles

Bulgac, A., I. Abdurrahman, K. Godbey and I. Stetcu. Fragment Intrinsic Spins and Fragments' Relative Orbital Angular Momentum in Nuclear Fission. 2022. *Physical Review Letters*. **128** (2): 022501. (LA-UR-21-27848 DOI: 10.1103/PhysRevLett.128.022501)

Bulgac, A., I. Abdurrahman, S. Jin, K. Godbey, N. Schunck and I. Stetcu. Fission fragments intrinsic spins and their correlations. Submitted to *Physical Review Letters*. (LA-UR-20-30404)

*M. M. Verriere, M. *., M. Verriere and M. R. Mumpower. Improvements to the macroscopic-microscopic approach of nuclear fission. 2021. *Physical Review C*. **103** (3): 034617. (LA-UR-20-26369 DOI: 10.1103/PhysRevC.103.034617)

Conference Papers

Mumpower, M. R., M. Verriere and J. Randrup. Macroscopic-microscopic fission yields. Presented at *FUSION20*. (Shizuoka, Japan, 2020-11-15 - 2020-11-15). (LA-UR-20-23186)

Reports

Angermeier, W., C. Barros, I. D. Dumitru, M. C. Holmes, J. R. Howard, S. R. Johnstun, G. B. King, J. T. Lindbloom, N. P. Lordi, A. Luu, S. E. Martinez, J. N. McBride, E. S. Nelluvelil, K. T. O'Dell, H. R. Pace, N. A. Poole, A. Ramkumar, S. M. Riedel, L. Singh, S. R. Venkat, D. A. Weatherred, J. Y. Wei, K. A. York, F. Yousuf, M. T. Andrews, D. M. Israel and J. A. Kulesza. Final Reports of the 2021 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-21-28941)

Sprouse, T. M., M. R. Mumpower, I. Stetcu and M. H. Verriere. HPC Requirements Addendum. Unpublished report. (LA-UR-20-26962)

Presentation Slides

Mumpower, M. R. Simultaneous calculation of fission fragment charge and mass yields with the Enhanced Finite-Range Liquid-Drop Model (eFRLDM). Presented at *Division of Nuclear Physics*, Los Alamos, New Mexico, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-30063)

Mumpower, M. R. KISS-II Review. . (LA-UR-22-20418)

Mumpower, M. R., I. Stetcu and T. M. Sprouse. A Dynamical Approach to Low-Energy Fission. . (LA-UR-21-31795)

Sprouse, T. M. Propagation of nuclear model uncertainties in science applications. Presented at *Workshop for Applied Nuclear Data Activities*, Los Alamos (virtual via WebEx), New Mexico, United States, 2021-01-25 - 2021-02-03. (LA-UR-21-20577)

Sprouse, T. M., M. R. Mumpower and I. Stetcu. A Dynamical Approach to Low-Energy Fission. . (LA-UR-22-21656)

Neutrino Physics with Short- and Long-baseline Experiments

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Project Description

Why do we live in a matter-dominated universe? The tiny, subatomic particles called "neutrinos" may hold the answer to this most sought-after question. The Deep Underground Neutrino Experiment (DUNE) which forms the United States flagship experiment aims to explore this by sending neutrinos over 800 miles from Illinois to South Dakota. Several neutrino experiments in the recent past reported anomalous results that indicate there maybe more than three types of neutrinos ("sterile" neutrinos), which if proved to be true will have significant implications to our current understanding of neutrinos. The Short-Baseline Neutrino (SBN) program at Fermilab is exploring existing hints to address this. Both of these efforts are part of the high energy physics mission for Department of Energy (DOE) Office of Science. The proposed research spans the DUNE and SBN experiments and significantly enhances their technical and physics capabilities towards achieving the above stated goals. Novel calibration techniques using a high-power laser system and a source of low energy neutral particles ("neutrons") are proposed in order to achieve the measurement precision needed for DUNE. At SBN, a rare particle production process will be studied to address the sterile neutrino question which will be a "breakthrough" result in neutrino physics.

Publications

Journal Articles

*Abi, B., R. Acciarri, M. A. Acero, G. Adamov, D. Adams, M. Adinolfi, Z. Ahmad, J. Ahmed, T. Alion, S. A. Monsalve, C. Alt, J. Anderson, C. Andreopoulos, M. P. Andrews, F. Andrianala, S. Andringa, A. Ankowski, M. Antonova, S. Antusch, A. Aranda-Fernandez, A. Ariga, L. O. Arnold, M. A. Arroyave, J. Asaadi, A. Aurisano, V. Aushev, D. Autiero, F. Azfar, H. Back, J. J. Back, C. Backhouse, P. Baesso, L. Bagby, R. Bajou, S. Balasubramanian, P. Baldi, B. Bambah, F. Barao, G. Barenboim, G. J. Barker, W. Barkhouse, C. Barnes, G. Barr, J. B. Monarca, N. Barros, J. L. Barrow, A. Bashyal, V. Basque, F. Bay, J. L. B. Alba, J. F. Beacom, E. Bechetoille, B. Behera, L. Bellantoni, G. Bellettini, V. Bellini, O. Beltramello, D. Belver, N. Benekos, F. B. Neves, J.

Berger, S. Berkman, P. Bernardini, R. M. Berner, H. Berns, S. Bertolucci, M. Betancourt, Y. Bezawada, M. Bhattacharjee, B. Bhuyan, S. Biagi, J. Bian, M. Biassoni, K. Biery, B. Bilki, M. Bishai, A. Bitadze, A. Blake, B. B. Siffert, F. D. M. Blaszczyk, G. C. Blazey, E. Blucher, J. Boissevain, S. Bolognesi, T. Bolton, M. Bonesini, M. Bongrand, F. Bonini, A. Booth, C. Booth, S. Bordoni, A. Borkum, T. Boschi, N. Bostan, P. Bour, S. B. Boyd, D. Boyden, J. Bracinik, D. Braga, D. Brailsford, A. Brandt, J. Bremer, C. Brew, E. Brianne, S. J. Brice, C. Brizzolari, C. Bromberg, G. Brooijmans, J. Brooke, A. Bross, G. Brunetti, N. Buchanan, H. Budd, D. Caiulo, P. Calafiura, J. Calcutt, M. Calin, S. Calvez, E. Calvo, L. Camilleri, A. Caminata, M. Campanelli, D. Caratelli, G. Carini, B. Carlus, P. Carniti, I. C. Terrazas, H. Carranza, A. Castillo, C. Castromonte, C. Cattadori, F. Cavalier, F. Cavanna, S. Centro, G. Cerati, A. Cervelli, A. C. Villanueva, M. Chalifour, C. Chang, E. Chardonnet, A. Chatterjee, S. Chattopadhyay, J. Chaves, H. Chen, M. Chen, Y. Chen, D. Cherdack, C. Chi, S. Childress, A. Chiriacescu, K. Cho, S. Choubey, A. Christensen, D. Christian, G. Christodoulou, E. Church, P. Clarke, T. E. Coan, A. G. Cocco, J. A. B. Coelho, E. Conley, J. M. Conrad, M. Convery, L. Corwin, P. Cotte, L. Cremaldi, L. Cremonesi, J. I. Crespo-Anad\xc3\xb3n, E. Cristaldo, R. Cross, C. Cuesta, Y. Cui, D. Cussans, M. Dabrowski, H. d. Motta, L. Da Silva Peres, C. David, Q. David, G. S. Davies, S. Davini, J. Dawson, K. De, R. M. De Almeida, P. Debbins, I. De Bonis, M. P. Decowski, A. de Gouv\xc3\xaaa, P. C. De Holanda, I. L. De Icaza Astiz, A. Deisting, P. De Jong, A. Delbart, D. Delepine, M. Delgado, A. Dell'Acqua, P. De Lurgio, J. R. T. de Mello Neto, D. M. DeMuth, S. Dennis, C. Densham, G. Deptuch, A. De Roeck, V. De Romeri, J. J. De Vries, R. Dharmapalan, M. Dias, F. Diaz, J. S. D\xc3\xadaz, S. D. Domizio, L. D. Giulio, P. Ding, L. D. Noto, C. Distefano, R. Diurba, M. Diwan, Z. Djurcic, N. Dokania, M. J. Dolinski, L. Domine, D. Douglas, F. Drielsma, D. Duchesneau, K. Duffy, P. Dunne, T. Durkin, H. Duyang, O. Dvornikov, D. A. Dwyer, A. S. Dyshkant, M. Eads, D. Edmunds, J. Eisch, S. Emery, A. Ereditato, C. O. Escobar, L. E. Sanchez, J. J. Evans, E. Ewart, A. C. Ezeribe, K. Fahey, A. Falcone, C. Farnese, Y. Farzan, J. Felix, E. Fernandez-Martinez, P. F. Menendez, F. Ferraro, L. Fields, A. Filkins, F. Filthaut, R. S. Fitzpatrick, W. Flanagan, B. Fleming, R. Flight, J. Fowler, W. Fox, J. Franc, K. Francis, D. Franco, J. Freeman, J. Freestone, J. Fried, A. Friedland, S. Fuess, I. Furic, A. P. Furmanski, A. Gago, H. Gallagher, A. Gallego-Ros, N. Gallice, V. Galymov, E. Gamberini, T. Gamble, R. Gandhi, R. Gandrajula, S. Gao, D. Garcia-Gamez, M. Garc\xc3\xada-Peris, S. Gardiner, D.

Gastler, G. Ge, B. Gelli, A. Gendotti, S. Gent, Z. Ghorbani-Moghaddam, D. Gibin, I. Gil-Botella, C. Girerd, A. K. Giri, D. Gnani, O. Gogota, M. Gold, S. Gollapinni, K. Gollwitzer, R. A. Gomes, L. V. G. Bermeo, L. S. G. Fajardo, F. Gonnella, J. A. Gonzalez-Cuevas, M. C. Goodman, O. Goodwin, S. Goswami, C. Gotti, E. Goudzovski, C. Grace, M. Graham, E. Gramellini, R. Gran, E. Granados, A. Grant, C. Grant, D. Gratieri, P. Green, S. Green, L. Greenler, M. Greenwood, J. Greer, W. C. Griffith, M. Groh, J. Grudzinski, K. Grzelak, W. Gu, V. Guarino, R. Guenette, A. Guglielmi, B. Guo, K. K. Guthikonda, R. Gutierrez, P. Guzowski, M. M. Guzzo, S. Gwon, A. Habig, A. Hackenburg, H. Hadavand, R. Haenni, A. Hahn, J. Haigh, J. Haiston, T. Hamernik, P. Hamilton, J. Han, K. Harder, D. A. Harris, J. Hartnell, T. Hasegawa, R. Hatcher, E. Hazen, A. Heavey, K. M. Heeger, J. Heise, K. Hennessy, S. Henry, M. A. H. Morquecho, K. Herner, L. Hertel, A. S. Hesam, J. Hewes, A. Higuera, T. Hill, S. J. Hillier, A. Himmel, J. Hoff, C. Hohl, A. Holin, E. Hoppe, G. A. Horton-Smith, M. Hostert, A. Hourlier, B. Howard, R. Howell, J. Huang, J. Huang, J. Hugon, G. Iles, N. Ilic, A. M. Iliescu, R. Illingworth, A. Ioannisian, R. Itay, A. Izmaylov, E. James, B. Jargowsky, F. Jediny, C. Jes\xc3\xb9s-Valls, X. Ji, L. Jiang, S. Jim\xc3\xa9nez, A. Jipa, A. Joglekar, C. Johnson, R. Johnson, B. Jones, S. Jones, C. K. Jung, T. Junk, Y. Jwa, M. Kabirnezhad, A. Kaboth, I. Kadenko, F. Kamiya, G. Karagiorgi, A. Karcher, M. Karolak, Y. Karyotakis, S. Kasai, S. P. Kasetti, L. Kashur, N. Kazaryan, E. Kearns, P. Keener, K. J. Kelly, E. Kemp, W. Ketchum, S. H. Kettell, M. Khabibullin, A. Khotjantsev, A. Khvedelidze, D. Kim, B. King, B. Kirby, M. Kirby, J. Klein, K. Koehler, L. W. Koerner, S. Kohn, P. P. Koller, M. Kordosky, T. Kosc, U. Kose, V. A. Kosteleck\xc3\xbd, K. Kothekar, F. Krennrich, I. Kreslo, Y. Kudenko, V. A. Kudryavtsev, S. Kulagin, J. Kumar, R. Kumar, C. Kuruppu, V. Kus, T. Kutter, A. Lambert, K. Lande, C. E. Lane, K. Lang, T. Langford, P. Lasorak, D. Last, C. Lastoria, A. Laundrie, A. Lawrence, I. Lazanu, R. LaZur, T. Le, J. Learned, P. LeBrun, G. L. Miotto, R. Lehnert, M. A. L. de Oliveira, M. Leitner, M. Leyton, L. Li, S. Li, S. W. Li, T. Li, Y. Li, H. Liao, C. S. Lin, S. Lin, A. Lister, B. R. Littlejohn, J. Liu, S. Lockwitz, T. Loew, M. Lokajicek, I. Lomidze, K. Long, K. Loo, D. Lorca, T. Lord, J. M. LoSecco, W. C. Louis, K. B. Luk, X. Luo, N. Lurkin, T. Lux, V. P. Luzio, D. MacFarland, A. A. Machado, P. Machado, C. T. Macias, J. R. Macier, A. Maddalena, P. Madigan, S. Magill, K. Mahn, A. Maio, J. A. Maloney, G. Mandrioli, J. Maneira, L. Manenti, S. Manly, A. Mann, K. Manolopoulos, M. M. Plata, A. Marchionni, W. Marciano, D. Marfatia, C. Mariani, J. Maricic, F. Marinho, A. D. Marino, M. Marshak, C. Marshall, J. Marshall, J. Marteau, J. Martin-Albo, N. Martinez, D. A. M. Caicedo, S. Martynenko, K. Mason, A. Mastbaum, M. Masud, S. Matsuno, J. Matthews, C. Mauger, N. Mauri, K. Mavrokoridis, R. Mazza, A. Mazzacane, E. Mazzucato, E. McCluskey, N. McConkey, K. S. McFarland, C. McGrew, A. McNab, A. Mefodiev, P. Mehta, P. Melas, M. Mellinato, O. Mena, S. Menary, H. Mendez, A. Menegolli, G. Meng, M. D. Messier, W. Metcalf, M. Mewes, H. Meyer, T. Miao, G. Michna, T. Miedema, J. Migenda, R. Milincic, W. Miller, J. Mills, C. Milne, O. Mineev, O. G. Miranda, S. Miryala, C. S. Mishra, S. R. Mishra, A. Mislivec, D. Mladenov, I. Mocioiu,

K. Moffat, N. Moggi, R. Mohanta, T. A. Mohayai, N. Mokhov, J. Molina, L. M. Bueno, A. Montanari, C. Montanari, D. Montanari, L. M. M. Zetina, J. Moon, M. Mooney, A. Moor, D. Moreno, B. Morgan, C. Morris, C. Mossey, E. Motuk, C. A. Moura, J. Mousseau, W. Mu, L. Mualem, J. Mueller, M. Muether, S. Mufson, F. Muheim, A. Muir, M. Mulhearn, H. Muramatsu, S. Murphy, J. Musser, J. Nachtman, S. Nagu, M. Nalbandyan, R. Nandakumar, D. Naples, S. Narita, D. Navas-Nicol\xc3\xa1s, N. Nayak, M. Nebot-Guinot, L. Necib, K. Negishi, J. K. Nelson, J. Nesbit, M. Nessi, D. Newbold, M. Newcomer, D. Newhart, R. Nichol, E. Niner, K. Nishimura, A. Norman, A. Norrick, R. Northrop, P. Novella, J. A. Nowak, M. Oberling, A. O. D. Campo, A. Olivier, Y. Onel, Y. Onishchuk, J. Ott, L. Pagani, S. Pakvasa, O. Palamara, S. Palestini, J. M. Paley, M. Pallavicini, C. Palomares, E. Pantic, V. Paolone, V. Papadimitriou, R. Papaleo, A. Papanestis, S. Paramesvaran, S. Parke, Z. Parsa, M. Parvu, S. Pascoli, L. Pasqualini, J. Pasternak, J. Pater, C. Patrick, L. Patrizii, R. B. Patterson, S. J. Patton, T. Patzak, A. Paudel, B. Paulos, L. Paulucci, Z. Pavlovic, G. Pawloski, D. Payne, V. Pec, S. J. M. Peeters, Y. Penichot, E. Pennacchio, A. Penzo, O. L. G. Peres, J. Perry, D. Pershey, G. Pessina, G. Petrillo, C. Petta, R. Petti, F. Piastra, L. Pickering, F. Pietropaolo, J. Pillow, J. Pinzino, R. Plunkett, R. Poling, X. Pons, N. Poonthottathil, S. Pordes, M. Potekhin, R. Potenza, B. V. K. S. Potukuchi, J. Pozimski, M. Pozzato, S. Prakash, T. Prakash, S. Prince, G. Prior, D. Pugnere, K. Qi, X. Qian, J. L. Raaf, R. Raboanary, V. Radeka, J. Rademacker, B. Radics, A. Rafique, E. Raguzin, M. Rai, M. Rajaoalisoa, I. Rakhno, H. T. Rakotondramanana, L. Rakotondravohitra, Y. A. Ramachers, R. Rameika, M. A. R. Delgado, B. Ramson, A. Rappoldi, G. Raselli, P. Ratoff, S. Ravat, H. Razafinime, J. S. Real, B. Rebel, D. Redondo, M. Reggiani-Guzzo, T. Rehak, J. Reichenbacher, S. D. Reitzner, A. Renshaw, S. Rescia, F. Resnati, A. Reynolds, G. Riccobene, L. C. J. Rice, K. Rielage, Y. Rigaut, D. Rivera, L. Rochester, M. Roda, P. Rodrigues, M. J. R. Alonso, J. R. Rondon, A. J. Roeth, H. Rogers, S. Rosauro-Alcaraz, M. Rossella, J. Rout, S. Roy, A. Rubbia, C. Rubbia, B. Russell, J. Russell, D. Ruterbories, R. Saakyan, S. Sacerdoti, T. Safford, N. Sahu, P. Sala, N. Samios, M. C. Sanchez, D. A. Sanders, D. Sankey, S. Santana, M. Santos-Maldonado, N. Saoulidou, P. Sapienza, C. Sarasty, I. Sarcevic, G. Savage, V. Savinov, A. Scaramelli, A. Scarff, A. Scarpelli, T. Schaffer, H. Schellman, P. Schlabach, D. Schmitz, K. Scholberg, A. Schukraft, E. Segreto, J. Sensenig, I. Seong, A. Sergi, F. Sergiampietri, D. Sgalaberna, M. H. Shaevitz, S. Shafaq, M. Shamma, H. R. Sharma, R. Sharma, T. Shaw, C. Shepherd-Themistocleous, S. Shin, D. Shooltz, R. Shrock, L. Simard, N. Simos, J. Sinclair, G. Sinev, J. Singh, J. Singh, V. Singh, R. Sipos, F. W. Sippach, G. Sirri, A. Sitraka, K. Siyeon, D. Smargianaki, A. Smith, A. Smith, E. Smith, P. Smith, J. Smolik, M. Smy, P. Snopok, M. S. Nunes, H. Sobel, M. Soderberg, C. J. S. Salinas, S. S\xc3\xb6ldner-Rembold, N. Solomey, V. Solovov, W. E. Sondheim, M. Sorel, J. Soto-Oton, A. Sousa, K. Soustruznik, F. Spagliardi, M. Spanu, J. Spitz, N. J. C. Spooner, K. Spurgeon, R. Staley, M. Stancari, L. Stanco, H. M. Steiner, J. Stewart, B. Stillwell, J. Stock, F. Stocker, T. Stokes, M. Strait, T. Strauss, S. Striganov, A. Stuart, D. Summers, A. Surdo, V. Susic, L. Suter, C. M. Sutera,

R. Svoboda, B. Szczerbinska, A. M. Szelc, R. Talaga, H. A. Tanaka, B. T. Oregui, A. Tapper, S. Tariq, E. Tatar, R. Tayloe, A. M. Teklu, M. Tenti, K. Terao, C. A. Ternes, F. Terranova, G. Testera, A. Thea, J. L. Thompson, C. Thorn, S. C. Timm, A. Tonazzo, M. Torti, M. Tortola, F. Tortorici, D. Totani, M. Toups, C. Touramanis, J. Trevor, W. H. Trzaska, Y. T. Tsai, Z. Tsamalaidze, K. V. Tsang, N. Tsverava, S. Tufanli, C. Tull, E. Tyley, M. Tzanov, M. A. Uchida, J. Urheim, T. Usher, M. R. Vagins, P. Vahle, G. A. Valdiviesso, E. Valencia, Z. Vallari, J. W. F. Valle, S. Vallecorsa, R. Van Berg, R. G. Van de Water, D. V. Forero, F. Varanini, D. Vargas, G. Varner, J. Vasel, G. Vasseur, K. Vaziri, S. Ventura, A. Verdugo, S. Vergani, M. A. Vermeulen, M. Verzocchi, H. V. de Souza, C. Vignoli, C. Vilela, B. Viren, T. Vrba, T. Wachala, A. V. Waldron, M. Wallbank, H. Wang, J. Wang, Y. Wang, Y. Wang, K. Warburton, D. Warner, M. Wascko, D. Waters, A. Watson, P. Weatherly, A. Weber, M. Weber, H. Wei, A. Weinstein, D. Wenman, M. Wetstein, M. R. While, A. White, L. H. Whitehead, D. Whittington, M. J. Wilking, C. Wilkinson, Z. Williams, F. Wilson, R. J. Wilson, J. Wolcott, T. Wongjirad, K. Wood, L. Wood, E. Worcester, M. Worcester, C. Wret, W. Wu, W. Wu, Y. Xiao, G. Yang, T. Yang, N. Yershov, K. Yonehara, T. Young, B. Yu, J. Yu, R. Zaki, J. Zalesak, L. Zambelli, B. Zamorano, A. Zani, L. Zazueta, G. P. Zeller, J. Zennamo, K. Zeug, C. Zhang, M. Zhao, E. Zhivun, G. Zhu, E. D. Zimmerman, M. Zito, S. Zucchelli, J. Zuklin, V. Zutshi and R. Zwaska. Long-baseline neutrino oscillation physics potential of the DUNE experiment. 2020. *The European Physical Journal C*. **80** (10): 978. (LA-UR-21-30819 DOI: 10.1140/epjc/s10052-020-08456-z)

*Gollapinni, S., DUNE Collaboration, R. G. Van De Water, W. C. I. Louis, W. E. Sondheim, K. R. Rielage and J. G. Boissevain. Volume III. DUNE far detector technical coordination. 2020. *Journal of Instrumentation*. **15** (08). (LA-UR-20-28752 DOI: 10.1088/1748-0221/15/08/T08009)

*Gollapinni, S., DUNE Collaboration, W. C. I. Louis, R. G. Van De Water, K. R. Rielage, W. E. Sondheim and J. G. Boissevain. Volume I. Introduction to DUNE. 2020. *Journal of Instrumentation*. **15** (08). (LA-UR-20-28748 DOI: 10.1088/1748-0221/15/08/T08008)

*Gollapinni, S., DUNE Collaboration, W. C. I. Louis, R. G. Van De Water, K. R. Rielage, W. E. Sondheim and J. G. Boissevain. Volume IV. The DUNE far detector single-phase technology. 2020. *Journal of Instrumentation*. **15** (08). (LA-UR-20-28763 DOI: 10.1088/1748-0221/15/08/T08010)

Gollapinni, S. and et al. DUNE Collaboration. First results on ProtoDUNE-SP liquid argon time projection chamber performance from a beam test at the CERN Neutrino Platform. Submitted to *Journal of Instrumentation 15 P12004*. (LA-UR-21-30820)

Reports

Gollapinni, S., G. Karagiorgi, M. R. Lonegran, W. C. I. Louis, R. G. Van De Water, A. Mogan, G. Yarbrough, W. Tang, MicroBooNE Collaboration and R. Fine. The MicroBooNE Single-Photon Low-Energy Excess Search. Unpublished report. (LA-UR-20-28825)

Gollapinni, S., R. D. Fine and et al. MicroBooNE Collaboration. Search for Neutrino-Induced Neutral Current Delta Radiative Decay in MicroBooNE and a First Test of the MiniBooNE Low Energy Excess Under a Single Photon Hypothesis (submitted to PRL). Unpublished report. (LA-UR-21-30821)

Gollapinni, S., R. D. Fine and et al. MicroBooNE Collaboration. Search for an Excess of Electron Neutrino Interactions in MicroBooNE Using Multiple Final State Topologies (submitted to PRL). Unpublished report. (LA-UR-21-30822)

Gollapinni, S., W. C. I. Louis, R. G. Van De Water, W. E. Sondheim, J. G. Boissevain, K. R. Rielage and DUNE Collaboration. Deep Underground Neutrino Experiment (DUNE), Far Detector Technical Design Report, Volume II: DUNE Physics. Unpublished report. (LA-UR-20-28836)

Presentation Slides

Gollapinni, S. Future Neutrino Experiments and Outlook. Presented at *40th International Conference on High Energy physics - ICHEP2020*, Prague, Czech Republic, 2020-07-28 - 2020-08-06. (LA-UR-21-22366)

Gollapinni, S. Unlocking the Mysteries of Neutrinos with the Deep Underground Neutrino Experiment. . (LA-UR-21-22367)

Gollapinni, S., A. Mogan and MicroBooNE Collaboration. Constraining the Neutral Current Pi0 Background for MicroBooNE's Single-Photon Search. Presented at *Fermilab New Perspective 2.0*, Batavia, Illinois, United States, 2020-08-24 - 2020-08-28. (LA-UR-20-28835)

Gollapinni, S., G. Karagiorgi and MicroBooNE Collaboration. Searches for New Physics with MicroBooNE. Presented at *XXIX International Conference on Neutrino Physics and Astrophysics (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28830)

Gollapinni, S., G. Yarbrough and MicroBooNE Collaboration. Systematic Studies for a Photon-like Low Energy Excess Search at MicroBooNE. Presented at *Fermilab New Perspectives 2.0*, Batavia, Illinois, United States, 2020-08-24 - 2020-08-28. (LA-UR-20-28834)

Gollapinni, S., M. Fani and et al. DUNE Collaboration. Status and Advances of the DUNE External Calibration Systems. Presented at *APS April Meeting 2021*, Virtual, District Of Columbia, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-30817)

Gollapinni, S., M. Fani and et al. DUNE Collaboration. Calibrating the world's largest LArTPC detector. Presented at *XIX International Workshop on Neutrino Telescopes*, Rome, Italy, 2021-02-18 - 2021-02-26. (LA-UR-21-30816)

Gollapinni, S., M. R. Lonegran and MicroBooNE Collaboration. Neutral Current Pi0 Rate Measurement with the

MicroBooNE Detector. Presented at *40th International Conference on High Energy Physics (ICHEP 2020)*, Prague, Czech Republic, 2020-07-28 - 2020-08-06. (LA-UR-20-28831)

Posters

Gollapinni, S., A. Mogan and MicroBooNE Collaboration. Constraining the Neutral Current Pi0 Background for MicroBooNE's Single-Photon Search. Presented at *53rd Fermilab Annual Users Meeting*, Batavia, Illinois, United States, 2020-08-10 - 2020-08-14. (LA-UR-20-28832)

Gollapinni, S., G. Yarbrough and MicroBooNE Collaboration. Systematic Studies for a Photon-like Low Energy Excess Search at MicroBooNE. Presented at *53rd Fermilab Annual Users Meeting*, Batavia, Illinois, United States, 2020-08-10 - 2020-08-14. (LA-UR-20-28833)

Gollapinni, S., G. Yarbrough and MicroBooNE Collaboration. Systematic Studies in the Gamma Low Energy Excess Analysis of the MicroBooNE Experiment. Presented at *XXIX INTERNATIONAL CONFERENCE ON NEUTRINO PHYSICS (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28828)

Gollapinni, S., W. Tang and MicroBooNE Collaboration. Detector Systematics Evaluation for the MicroBooNE Single Photon Analysis. Presented at *XXIX INTERNATIONAL CONFERENCE ON NEUTRINO PHYSICS (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28928)

Mogan, A., S. Gollapinni and MicroBooNE Collaboration. Constraining the Neutral Current Pi0 Background for MicroBooNE's Single-Photon Search. Presented at *XXIX INTERNATIONAL CONFERENCE ON NEUTRINO PHYSICS (Neutrino 2020)*, Chicago, Illinois, United States, 2020-06-22 - 2020-07-02. (LA-UR-20-28826)

Laser Cooling and Trapping Beryllium

Xinxin Zhao
20210044ER

Project Description

The ability to laser cool and trap beryllium isotopes has exciting applications involving both the Los Alamos National Laboratory (LANL) nuclear forensics mission and fundamental science. For the LANL nuclear forensics mission, the beryllium 10 (Be-10) isotope can be used to reveal information about the carbon mass of a nuclear device. In fundamental science, Be-7 radioisotopes can be used to probe the existence of kiloelectron volt (keV)-mass sterile neutrinos with unprecedented sensitivity. Discovery of sterile neutrinos will have profound implications on three of the most urgent open problems in physics: the nature of neutrino masses, the nature of dark matter, and the origin of the matter-antimatter asymmetry in the universe. The common challenge in both emerging applications is trapping neutral Be atoms, and we propose to demonstrate the first Magneto-Optical Trapping of Be atoms to solve it.

Publications

Presentation Slides

Ahrens, J. P. LDRD ISTI Proposal Review (20210527CR) Information Science and Technology Institute (ISTI): Foundational Research in Information Science and Technology. . (LA-UR-20-28422)

Compact High-Gradient Booster for Enhanced Proton Radiography

Sergey Kurennoy
20210048ER

Project Description

Our project aims to develop a compact linear accelerator (< 50 meter) to boost the beam energy of protons at Los Alamos Neutron Science Center (LANSCE) from 0.8 gigaelectronvolt (GeV), provided by the existing accelerator, to 3 GeV. This energy increase will improve the proton radiography resolution 10 times. The compact booster will be based on high-gradient cavities that we will adapt for proton beams. This enhancement of proton radiography capability at LANSCE, which can be accomplished without significant changes to the existing infrastructure, will benefit National Nuclear Security Administration Defense Programs and fundamental materials research. High-gradient structures potentially can provide compact proton accelerators for cancer therapy and homeland defense.

Publications

Conference Papers

Kurennoy, S. S. and Y. K. Batygin. High-Gradient Booster for Enhanced Proton Radiography at LANSCE. Presented at *12th International Particle Accelerator Conference - IPAC'21(virtual)*. (Campinas, Brazil, 2021-05-24 - 2021-05-28). (LA-UR-21-24609)

Presentation Slides

Batygin, Y. K. and S. S. Kurennoy. Progress in Design of 3-GeV High-Gradient pRad Booster for LANSCE. Presented at *LANSCE Futures Spring 2021 Workshop Series: Dynamic Radiography*, Los Alamos (virtual format), New Mexico, United States, 2021-04-05 - 2021-04-06. (LA-UR-21-23157)

Ceramic Enhanced Accelerator Structures

Leanne Duffy
20210083ER

Project Description

Pillbox accelerator cavities are used everywhere because they are inexpensive, reliable, work over a huge frequency range, and accelerate electron beams as well as proton and ion beams. Our innovative new cavity designs will increase efficiency by 40% over normal conducting accelerator cavities without compromising performance criteria. This technology will also improve delivery of high-brightness electron beams, a crucial improvement for next generation large-scale accelerator projects such as x-ray light sources and linear colliders. Upgraded linac structures for the Los Alamos Neutron Science Center (LANSCE) will be of interest to the National Nuclear Security Administration as a risk mitigation and capability enhancement strategy. Development of intrinsically wake-damped, high-efficiency structures is expected to be of high interest to High Energy Physics and Basic Energy Sciences within Department of Energy-Office of Science, via direct impact to the length and power consumption, and therefore cost, of next-generation research and user facility accelerators.

Publications

Presentation Slides

Nichols, K., J. W. I. Lewellen, L. D. Duffy, M. A. Holloway, E. I. Simakov, J. Upadhyay and F. L. Krawczyk. Employing High Epsilon Dielectric Materials for Enhancing Cu Accelerator. Presented at *Snowmass miniWorkshop on Innovative Design*, Chicago, Illinois, United States, 2021-01-26 - 2021-01-26. (LA-UR-21-20673)

Neutralizer-Based Longitudinal Bunch Profile Measurement

Heather Andrews
20210156ER

Project Description

High-power particle accelerators are foundational tools used to support missions that address national security challenges, in particular stockpile stewardship. This work addresses two related challenges associated with such accelerators: making high-resolution measurements of the accelerator's particle beam properties while it is in operation; and diagnosing conditions that can result in beam loss inside, and subsequent damage to, the accelerator. Such machines are also useful for basic science research, particularly in nuclear and high-energy physics, where they serve as neutrino factories, spallation neutron sources, exotic beam drivers, etc.; this work will help address the operating challenges of all such machines.

Deconstructing the Cabibbo Angle Anomaly

Emanuele Mereghetti
20210190ER

Project Description

This project will develop the theoretical and computational tools needed to probe the fundamental constituents of matter and their interactions through precision measurements of neutron and nuclear beta disintegrations. This project is very timely due to the recent emergence of tensions between measurements and the interpretation in terms of the known physical laws governing subatomic physics. The project goal is to improve the theoretical precision of beta disintegrations of nuclei and thus assess the possibility that new phenomena might impact them. Furthering the understanding of matters constituents and interactions and possibly discovering new ones is a significant component of the Department of Energy (DOE) Office of Science (Nuclear Physics) mission, as elucidated in the latest Long Range Plan by the Nuclear Science Advisory Committee. The success of this project would have a strong positive impact on the Los Alamos and broader DOE experimental program in precision beta decay studies.

Publications

Journal Articles

Cirigliano, V., D. Bryman, A. Crivellin and G. Inguglia. Testing Lepton Flavor Universality Violation in the Charged Current with Kaon, Pion, Tau and Beta Decays. Submitted to *Annual Review of Nuclear and Particle Science*. (LA-UR-21-30608)

Cirigliano, V., D. Diaz-Calderon, A. Falkowski, A. Rodriguez-Sanchez and M. Gonzalez-Alonso. Semileptonic tau decays beyond the Standard Model. Submitted to *Journal of High Energy Physics*. (LA-UR-21-31791)

Cirigliano, V., E. Mereghetti, L. M. Hayen, A. Walker-Loud and J. de Vries. Radiative correction to neutron decay in effective field theory. Submitted to *Physical Review Letters*. (LA-UR-21-31960)

Mereghetti, E., G. King, A. Baroni, V. Cirigliano, S. Gandolfi, L. Hayen, S. Pastore and M. Piarulli. Ab initio calculation of the beta decay spectrum of 6He. Submitted to *Physical Review C*. (LA-UR-21-31938)

Mereghetti, E., K. Fuyuto, V. Cirigliano, W. Dekens, J. de Vries and R. Ruiz. The muon's anomalous magnetic moment in nuSMEFT. Submitted to *Physical Review D*. (LA-UR-21-24456)

Mereghetti, E., R. Boughezal and F. Petriello. Dilepton production in the SMEFT at O(1/Lambda^4). Submitted to *Journal of High Energy Physics*. (LA-UR-21-25379)

Mereghetti, E., V. Cirigliano, W. Dekens, J. de Vries and M. Hoferichter. Towards complete leading order predictions for neutrinoless double beta decay. Submitted to *Physical Review Letters*. (LA-UR-20-30355)

Tomalak, O. S., Q. Chen, R. J. Hill and K. S. McFarland. QED radiative corrections to neutrino-nucleon elastic scattering. Submitted to *Physical Review Letters*. (LA-UR-21-27844)

Presentation Slides

Cirigliano, V. and E. Mereghetti. Deconstructing the Cabibbo angle anomaly. . (LA-UR-21-31961)

Fuyuto, K. Searches for violations of fundamental symmetries. . (LA-UR-22-20417)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-20967)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22082)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22446)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22469)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22561)

Tomalak, O. S. Axial and pseudoscalar form factors from charged-current neutrino-nucleon elastic scattering. Presented at *2021 Fall Meeting of the APS DNP, virtual*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-11. (LA-UR-21-29985)

Posters

Tomalak, O. S. QED corrections to charged-current neutrino-nucleon elastic scattering. Presented at *PANIC 2021:*

From Solids to Plasmas: A Universal Approach to Ab Initio Modeling Across Temperature Regimes

Alexander White
20210233ER

Project Description

Predictive modeling is critical for understanding complex systems under extreme conditions, where experimental results can be expensive to obtain or difficult to interpret. Successfully modeling such systems requires accurate calculation of material properties, such as equation of state, mass transport and conductivity. Kohn Sham Density Functional Theory (KS-DFT), based on first-principle quantum mechanics, has become the premier method for the calculation of these properties. However, for extreme conditions, these predictive calculations are often numerically intractable. This is because the computational costs of these calculations grow with both temperature and system size. This necessitates a patchwork of more approximate methods for different regimes and often leads to inconsistent results. Our novel approach is based on the unification of the traditional deterministic algorithm for KS-DFT with a recently developed stochastic algorithm to achieve the same accuracy at lower costs. This universal DFT algorithm allows for optimization of computational costs based on desired precision, available computational resources, system temperatures, densities, and size. We are delivering the theory, initial applications, and software required to motivate and facilitate the widespread adoption of our new algorithm. This will constitute a significant leap in nations ability to model the microscopic physics of matter at extreme conditions.

Publications

Journal Articles

Malko, S., W. Cayzac, V. Ospina-Bohorquez, K. Bhutwala, M. Bailly-Grandvaux, C. McGuffey, R. Fedosejevs, X. Vaisseau, A. Tauschwitz, J. Apinaniz, D. De Luis, G. Gatti, M. Huault, J. Perez-Hermandez, S. Hu, A. J. White, L. A. Collins, P. Neumayer, G. Faussurier, J. Vorberger, G. Prestopino, C. Verona, J. Santos, D. Batani, F. N. Beg and L. Volpe. Proton stopping measurements at low velocity in warm dense carbon. Submitted to *Nature Communications*. (LA-UR-21-28294)

Nichols, K. A., S. Hu, L. A. Collins and A. J. White. Mixed Stochastic-Deterministic Time-Dependent Density Functional Theory: Application to Stopping Power of Warm Dense Carbon. Submitted to *Journal of Physics: Condensed Matter*. (LA-UR-21-31679)

Presentation Slides

Nichols, K. A., A. J. White, L. A. Collins and S. Hu. Investigating the Stopping Power of Warm Dense Plasmas using Time-Dependent Mixed Density-Functional Theory (TD-mDFT). Presented at *APS DPP*, Pittsburgh, Pennsylvania, United States, 2021-11-09 - 2021-11-09. (LA-UR-21-30711)

White, A. J., L. A. Collins, K. A. Nichols and S. Hu. Time-Dependent Mixed Deterministic-Stochastic Kohn Sham Density Functional Theory for Matter in Extreme Conditions. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21867)

Posters

White, A. J. Nonequilibrium Dynamics of Materials in Extreme Conditions : Ab initio simulation of stopping of high energy projectiles by warm dense matter. . (LA-UR-21-29192)

Multiscale method for fluid-kinetic coupling in ocean-world jet simulations

Daniel Livescu
20210298ER

Project Description

Many problems of importance to Department of Energy (DOE)/National Nuclear Security Administration (NNSA) cover regimes where atomistic effects are important, but at scales where kinetic calculations are not possible. Examples extend from flows at microscales in Inertial Confinement Fusion, to stockpile applications, to earth's magnetic field and space weather, and to astrophysics. There is an urgent need for accurate calculations of such applications, and this is currently a very active area of research with a plethora of multiscale approaches, which also underlines the difficulty of the problem. Our multiscale method relies on a very promising approach, ensuring premier high-fidelity, but computationally efficient calculations. The application we have chosen to demonstrate the approach is timely in light of the National Aeronautics and Space Administration's (NASA's) planned space missions, but lacks any pertinent calculation to date. Thus, our first ever calculations of Enceladus/Europa water jets will guide future space missions by helping understand jet source conditions and also estimating forces/stresses on probes/landers expected to be dropped in those jets. In addition, the cost-efficient multiscale method developed in this work could facilitate spatially multi-dimensional simulations coupling hydrodynamic phenomena with dense plasma and kinetic effects encountered in DOE/NNSA specific applications.

Publications

Journal Articles

Sharan, N. and J. Bellan. Investigation of high-pressure turbulent jets using direct numerical simulation. Submitted to *Journal of Fluid Mechanics*. (LA-UR-21-26442)

Wei, T. and D. Livescu. Scaling of the mean transverse flow and Reynolds shear stress in turbulent plane jet. Submitted to *Physics of Fluids*. (LA-UR-21-20834)

Wei, T. and D. Livescu. Scaling analysis of turbulent planar plume. Submitted to *Physics of Fluids*. (LA-UR-21-23862)

Presentation Slides

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Objective discovery of fluid dynamical regimes with unsupervised machine learning. Presented at *American Physical Society Division of Fluid Dynamics Fall Meeting*, Phoenix, Arizona, United States, 2021-11-22 - 2021-11-22. (LA-UR-21-31365)

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Objective discovery of dominant dynamical regimes. Presented at *Machine Learning for Climate (Kavli Institute for Theoretical Physics)*, Santa Barbara, California, United States, 2021-11-01 - 2021-11-04. (LA-UR-21-31428)

Kaiser, B. E., J. A. Saenz, M. Sonnewald and D. Livescu. Objective discovery of dominant dynamical regimes. Presented at *Machine Learning for Climate (Kavli Institute for Theoretical Physics)*, Santa Barbara, California, United States, 2021-11-01 - 2021-11-04. (LA-UR-21-31437)

Towards Actinide Scattering Measurements at the Los Alamos Neutron Science Center

Keegan Kelly
20210329ER

Project Description

Neutron scattering is the most common neutron reaction on fissionable and non-fissionable nuclei, and thus information on these poorly-known reactions is essential for descriptions of fission-driven systems. We aim to provide unparalleled measurements of these reactions with highly-restrictive cross-reaction correlations to provide a breakthrough in the accuracy with which Department of Energy/National Nuclear Security Administration mission-relevant systems can be studied. Additionally, the never-before-measured correlations between these reactions and other neutron-induced reactions will severely limit the extent to which nuclear data libraries can be varied to match criticality benchmarks, thereby potentially revealing other lingering and previously unknown nuclear data errors in other reactions of interest.

Publications

Journal Articles

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Correlated n-\xce\xb3 Angular Distributions from the 12C(n,n#1) Reaction for Incident Neutron Energies from 6.5–16.5 MeV. Submitted to *Physical Review C*. (LA-UR-21-21204)

Presentation Slides

Bennett, E. A. Direct Measurements of Neutron Scattering at LANSCE. Presented at *Low Energy Community Meeting*, Los Alamos, New Mexico, United States, 2021-08-09 - 2021-08-11. (LA-UR-21-28103)

Bennett, E. A. Design and Simulation of a Next-Generation Dual n-gamma Detector Array at Los Alamos National Laboratory. Presented at *Division of Nuclear Physics Conference 2021*, Boston, Massachusetts, United States, 2021-10-11 - 2021-10-14. (LA-UR-21-30190)

Kelly, K. J. Development in Neutron Scattering at WNR using Dual n-gamma Detection. . (LA-UR-21-23850)

Kelly, K. J. Neutron Scattering and Future Experimental Capabilities at WNR. Presented at *LANSCE Futures Spring Workshop 2021: Nuclear Science*, LOS ALAMOS, New Mexico, United States, 2021-05-10 - 2021-05-11. (LA-UR-21-24514)

Kelly, K. J. LANL ``What Do We Get'' Report. . (LA-UR-22-20570)

Kelly, K. J., M. A. Mosby and T. Kawano. Dual n-gamma Measurement of the 235U(n,3n) Cross Section. . (LA-UR-21-29859)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell, E. A. Bennett and M. W. Paris. LANL Updates on Chi-Nu and Neutron Scattering. Presented at *CSEWG 2021*, Upton, New York, United States, 2021-11-15 - 2021-11-19. (LA-UR-21-31496)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell, M. W. Paris and E. A. Bennett. White Source n-gamma Coincidence Measurements of gamma-Production Cross Sections at LANSCE. . (LA-UR-21-30669)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. LANSCE Experimental Updates II: Neutron Scattering at WNR. Presented at *2020 Cross Section Evaluation Working Group*, Upton, New York, United States, 2020-11-30 - 2020-12-04. (LA-UR-20-29952)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Development of Dual n-gamma Techniques at the Los Alamos Neutron Science Center. Presented at *SORMAWest 2021*, N/A, New Mexico, United States, 2021-05-14 - 2021-05-21. (LA-UR-21-24477)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Prompt Fission Neutron Detection and Neutron Scattering Measurements at WNR FP15L. . (LA-UR-21-30485)

Posters

Bennett, E. A., K. J. Kelly, M. J. Devlin and J. M. O'Donnell. Design and Simulation of a Next-Generation Dual n-gamma Detector Array at LANL. Presented at *IEEE Symposium on Radiation Measurements and Applications (SORMA West)*, Berkeley, California, United States, 2021-05-19 - 2021-05-28. (LA-UR-21-24796)

Unmasking Dark Matter with the Migdal Effect

Steven Elliott
20210499ER

Project Description

This effort will develop a directionally sensitive measurement for neutrons. The driving goal of the experiment is the full understanding of existing and proposed dark matter experiments, a major set of investments by Department of Energy (DOE). While it is conceivable that the technology could be used for neutron detection, the underlying purpose is the measurement of a key atomic-nuclear physics effect that is the foundation of many dark matter searches.

Publications

Presentation Slides

Colgan, J. P. Unmasking Dark Matter with the migdal effect. . (LA-UR-22-21509)

Massarczyk, R. Chasing neutrinos a mile underground. . (LA-UR-20-29252)

Posters

Colgan, J. P. and M. S. Pindzola. Neutron-impact ionization of the carbon atom. Presented at *DAMOP 2021*, Online, New Mexico, United States, 2021-05-31 - 2021-05-31. (LA-UR-21-25164)

Development of Superconducting Accelerating Cavities with Magnesium Diboride (MgB2) Coating

Tsuyoshi Tajima
20210720ER

Project Description

This project will develop a technique to coat a particle accelerator structure with magnesium diboride (MgB2) , a promising superconductor that has a great potential to reduce the size and construction cost compared to the accelerator based on the conventional superconductor niobium (Nb) since it can become superconductive at a >4 times higher temperature (39 Kelvin vs. 9 Kelvin). If successful, an MgB2 coated accelerator can be a small module with a small cooler so-called a cryocooler instead of using liquid helium that requires a large facility to re-liquefy the evaporated helium and circulate the liquid. This compact MgB2 accelerator could be used for various national security missions such space missions, active interrogation for border security, and upgrades of the Los Alamos Neutron Science Center (LANSCE) accelerator for stockpile stewardship. In addition, it can provide an economic solution to the envisioned x-ray free-electron laser based on a high-energy electron accelerator as a part of future Dynamic Mesoscale Materials Science Capability (DMMSC) for Department of Energy / National Nuclear Security Administration.

Publications

Conference Papers

Pizzol, P., I. Nekrashevich, L. Civale, A. Poudel, H. R. Salazar, D. Kelly, R. K. Schulze and T. Tajima. PROGRESS OF MgB2 DEPOSITION TECHNIQUE FOR SRF CAVITIES AT LANL. Presented at *SRF 2021*. (Grand Rapids, Michigan, United States, 2021-06-28 - 2021-07-02). (LA-UR-21-25776)

Posters

Pizzol, P., A. Poudel, I. Nekrashevich, L. Civale, D. Kelly, R. K. Schulze and T. Tajima. PROGRESS OF MgB2 DEPOSITION TECHNIQUE FOR SRF CAVITIES AT LANL. Presented at *SRF 2021*, Grand Rapids, Michigan, United States, 2021-06-28 - 2021-07-02. (LA-UR-21-25818)

Studying Double Neutron Capture for Forensics Applications

Aaron Couture
20210773ER

Project Description

In the event of a nuclear detonation, it is critical that the United States be positioned to rapidly and accurately determine how the device was designed, an effort broadly known as nuclear forensics. Radioactive traces observable after the detonation can reveal information about both the conditions of the detonation and the materials present in the nuclear device. But the fidelity of those determinations is only as good as our knowledge of the reaction channels. A new measurement facility, the Soreq Applied Research Accelerator Facility, offers the chance to study reactions on unstable isotopes in a combined effort to both make and measure the isotope in one experiment. This effort will study exactly which isotopes could be measured with this new facility, and look at which measurements would be most important to pursue in the coming years to meet our strategic objectives for nuclear forensics.

Enabling High-Temperature and High-Energy-Density Physics Using X-Ray Free Electron Lasers

Steven Batha
20210789ER

Project Description

Ever more precise experiments and measurements must be made to validate the computer simulation codes we use in our national security enterprise. Newly created Department of Energy facilities, such as the fourth-generation light sources, especially the x-ray free electron lasers (XFELs), provide a tremendous advance in the precision that can be attained in certain classes of experiments. This project will develop software that will be used to design experiments so that the accuracy of the measurements can be determined before the experiment is performed. Knowing the uncertainty in the measurements will then quantify the uncertainty in the simulation codes. This will allow for identification of areas where the codes need to be improved. This project will also develop and mature concepts for making large quantities of precision targets that are used to create the experimental conditions, both cheaply and reproducibly.

Advancing the Frontiers of High-Precision Quantum Chromodynamics (QCD) with Machine-Learning-Enhanced Monte Carlo Algorithms

Christopher Lee
20210804ER

Project Description

We apply computational advances based on machine learning to the high-precision prediction of cross sections mediated by the strong interaction in high-energy collisions of electrons, positrons, and protons. Being able to predict the products of these collisions to high accuracy allows them to be used to study the structure of matter and the forces between them in exquisite detail, teaching us about the fundamental nature of matter and evolution of the universe. Our research could enhance the speed and accuracy of computations of these cross sections by factors of 100 or 1000, making a huge impact on the efficiency and range of research on the strong interaction that would be made possible. This would enhance our ability to meet the high-priority scientific goals of the Department of Energy (DOE) Office of Science as expressed in its Long-Range Plans for nuclear science and high-energy physics, to probe the structure of protons, the fundamental forces between their constituents, and search for signs of new physics beyond the Standard Model. It would bolster United States (US) scientific leadership in large international scientific collaborations such as the upcoming Electron-Ion Collider project.

Publications

Journal Articles

*Yoon, B. A machine learning approach for efficient multi-dimensional integration. 2021. *Scientific Reports*. **11** (1): 18965. (LA-UR-20-27161 DOI: 10.1038/s41598-021-98392-z)

Presentation Slides

Lee, C., B. Yan, B. Yoon, G. Bell, Y. Makris and J. Talbert. Angularities, gaps, and \\alpha_s. Presented at *World SCET 2021*, Cambridge, Massachusetts, United States, 2021-04-19 - 2021-04-23. (LA-UR-21-23742)

Lee, C., B. Yoon, B. Yan, Y. Makris, J. Talbert and G. Bell. Event shape tails and alpha_s. Presented at *INT Workshop on Probing QCD at High Energy and Density with Jets*, Seattle, Washington, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-27921)

Ultrafast Optical Neutron Detector

Kevin Henderson
20210829ER

Project Description

The success of this project could have a big impact on nuclear forensics, characterization of radiation damage, and other programs in Los Alamos National Laboratory (LANL), Department of Energy (DOE), Department of Homeland Security (DHS), and Department of Defense (DOD). But most importantly, this proposed neutron detector is a competitive alternative to Helium-3 neutron detectors which are threatened by a shortage of Helium-3. Alternatives like this proposed detector are especially vital to many DHS and DOE programs.

A Search of Weakly-Interacting Dark Matter in the Low Mass Region

Zhaowen Tang
20210834ER

Project Description

Direct detection of dark matter (DM) is an important area of focus for the Department of Energy (DOE) office of science, high energy physics program office. Our dark matter detection idea has a unique opportunity to probe a currently unexplored mass region for both spin independent and spin dependent DM. The result of this project will answer key questions regarding a hydrocarbon-based DM detector, and open up possibility for a prototype experiment that would probe a previously inaccessible parameter space.

Novel Seeding Method for Compact Terahertz (THz) Free Electron Lasers

MD Zuboraj
20210847ER

Project Description

The project addresses several national security challenges: 1. Everyone knows about millimeter-wave security screening at airports (30-300 gigahertz (GHz)). Unlike those mm-wave imaging, Terahertz (THz) imaging (300-3000GHz) can be used anywhere to detect concealed chemical weapons, drugs and improvised explosive devices (IED). Right now, the state-of-the-art THz sources provide too little power for accurate signal detection and imaging. This project aims to address this problem. A free electron laser (FEL) system can provide several tens of watts of THz power that can be used for security imaging, short-range radars and high speed surveillance systems. 2. The project directly studies the physics involved in miniaturization of large FEL systems, thereby addressing the Department of Energy's (DOE's) mission on compact accelerator systems. These compact accelerators can be used for food safety and medical purposes such as cancer detection, destroying cancer cells etc. 3. The study of the seeding method directly relates to the Laboratory's Dynamics Mesoscale Material Science Capability (DMMSC). The seeding method can be generalized to x-ray FEL system if proven successful. This addresses the DOE/National Nuclear Security Administration mission on making compact X-ray sources and detectors.

Production of Shaped Electron Bunches with Diamond Field Emitter Array Cathodes

Evgenya Simakov
20180078ER

Project Description

This project has the potential to advance the diamond field emitter array (DFEA) cathode technology and make it suitable for a number of national security applications that require high current, high power electron beams. This includes compact accelerators for warfighter support (e.g. small weaponized free-electron lasers), active interrogation, environmental remediation, and multi-megawatt X-ray sources. DFEAs present the most natural means of producing very high current electron bunches: they produce electron beams from the tips of diamond pyramids that can be fabricated and arranged in customized arbitrary patterns to suit the particular application, they generate a very stable and robust electron beam, and they produce the extremely high current densities that are necessary for obtaining multi-nano-Coulomb bunches.

Technical Outcomes

The primary outcome of this work was successful demonstration of shaped electron beam production from diamond field emitter array cathodes. The beams were produced in a 1.3 gigahertz (GHz) radio frequency (RF) injector. The team demonstrated production and transport along the 2.5 meter long beamline of two distinct beam shapes: a beam consisting of several shaped beamlets produced by a sparse array of diamond pyramids, and a triangular beam produced by a dense array.

Publications

Journal Articles

*Andrews, H., K. Nichols, K. Dongsung, E. I. Simakov, S. Antipov, C. Gongxiaohui, M. Conde, D. Doran, H. Gwanghui, L. Wanming, J. Power, S. Jiahang and E. Wisniewski. Shaped Beams from Diamond Field-Emitter Array Cathodes. 2020. *IEEE Transactions on Plasma Science*. **48** (7): 2671-2675. (LA-UR-19-31870 DOI: 10.1109/TPS.2020.2984156)

*Kim, D., H. L. Andrews, B. K. Choi, R. L. Fleming, C. Huang, T. J. T. Kwan, J. W. I. Lewellen, K. Nichols, V. Pavlenko and E. I. Simakov. Divergence study and emittance measurements for the electron beam emitted from a diamond pyramid. 2020. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **953**: 163055. (LA-UR-19-30904 DOI: 10.1016/j.nima.2019.163055)

*Nichols, K. E., H. L. Andrews, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. E. Wisniewski, S. P. Antipov and G. Chen. Demonstration of transport of a patterned electron beam produced by diamond pyramid cathode in an rf gun. 2020. *Applied Physics Letters*. **116** (2): 23502. (LA-UR-19-23845 DOI: 10.1063/1.5128109)

Schneider, M. E., E. J. Jevarjian and S. V. Baryshev. FEgen (v.1): Field Emission Distribution Generator Freeware Based on Fowler-Nordheim Equation. Submitted to *Review of Scientific Instruments note*. (LA-UR-21-25780)

Schneider, M. E., E. Jevarjian, J. Shao and S. V. Baryshev. FEbeam: Cavity and Electron Emission Data Conversion, Processing and Analysis. A Freeware Toolkit for RF Injectors. Submitted to *Review of Scientific Instruments*. (LA-UR-21-22493)

Schneider, M. E., E. Jevarjian, T. Nikhar, T. Posos, W. Liu, J. Shao and S. Baryshev. Ampere-class bright field emission cathode operated at 100 MV/m. 2021. *Physical Review Accelerators and Beams*. **24** (12): 123401. (LA-UR-21-20804 DOI: 10.1103/PhysRevAccelBeams.24.123401)

Conference Papers

Andrews, H. L., K. Nichols, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. Wisniewski, S. Antipov and G. Chen. Diamond Field Emitter Array Cathode Experimental Tests in RF Gun. Presented at *NAPAC 2019*. (Lansing, Michigan, United States, 2019-09-01 - 2019-09-06). (LA-UR-19-29010)

Nichols, K., E. I. Simakov, D. Shchegolkov and H. L. Andrews. MODELING OF DIAMOND FIELD EMITTER ARRAYS FOR SHAPED ELECTRON BEAM PRODUCTION. Presented at *IPAC*

18. (Vancouver, Canada, 2018-04-29 - 2018-05-04). (LA-UR-18-23590)

Nichols, K., H. L. Andrews, D. Kim, E. I. Simakov, M. Conde, D. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. E. Wisniewski, S. Antipov and G. Chen. Experimental Results of Dense Array Diamond Field Emitters in RF Gun. Presented at *IPAC*. (Melbourne, Australia, 2019-05-19 - 2019-05-24). (LA-UR-19-24470)

Pavlenko, V., D. Kim, H. L. Andrews, D. V. Gorelov and E. I. Simakov. Strong-Field Photoemission Experiment using Diamond Field Emitter Arrays. Presented at *AAC 2020*. (Berkeley, California, United States, 2020-11-18 - 2021-02-03). (LA-UR-21-21462)

Simakov, E. I., H. L. Andrews, C. Huang, T. J. T. Kwan, D. Kim, J. W. I. Lewellen, K. Nichols and V. Pavlenko. High current field emission electron sources for linear colliders and RF source applications. Presented at *Particle Physics Community Planning Exercise (Snowmass 2021)*. (Seattle, Washington, United States, 2021-07-11 - 2021-07-11). (LA-UR-20-26499)

Presentation Slides

Andrews, H. L., D. Kim, K. Nichols, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. E. Wisneiwski, S. P. Antipov and G. Chen. Shaped beams from Diamond Field-Emitter Array Cathodes. Presented at *PPPS2019*, orlando, Florida, United States, 2019-06-23 - 2019-06-28. (LA-UR-19-25996)

Andrews, H. L., K. Nichols, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. Wisniewski, S. Anitipov and G. Chen. Shaped Beams from Diamond Field-Emitter Array Cathodes. Presented at *NAPAC 2019*, Lansing, Michigan, United States, 2019-09-01 - 2019-09-06. (LA-UR-19-28834)

Nichols, K., H. L. Andrews, E. I. Simakov, D. Kim, M. Conde, D. S. Doran, G. Ha, W. Liu, J. G. Power, J. Shao, C. Whiteford, E. Wisniewski, S. Antipov and G. Chen. Diamond Field-Emitter Array Cathodes. Presented at *Advanced Accelerator Conference Seminar Series*, Chicago, Illinois, United States, 2021-01-13 - 2021-01-13. (LA-UR-21-20273)

Schneider, M. E., E. Jevarjian, J. Shao, T. Posos, T. Nikhar, W. Lui and B. Sergey. Demonstration of Ampere-class Field Emission Cathodes Operating at 100 MV/M And Excess of Child-Langmuir Law. Presented at *International particle accelerator conference*, Campinas, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24613)

Schneider, M. E., E. Jevarjian, J. Shao, T. Posos, T. Nikhar, W. Lui and S. V. Baryshev. Demonstration of Ampere-class Field Emission Cathodes Operating at 100 MV/M and Excess of Child-Langmuir Law. Presented at *Advanced accelerator concepts 2020: seminar series*, online, California, United States, 2021-01-13 - 2021-01-13. (LA-UR-21-20177)

Schneider, M. E., H. L. Andrews, S. V. Baryshev, D. Kim, K. Nichols, T. Posos and E. I. Simakov. Principal Mechanisms For The Production Of Pattern Beams Using Diamond Field Emission Array Cathodes For Braided Beam Applications. Presented at *Jared Maxson's group meeting*, Ithaca, New York, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22290)

Simakov, E. I., H. L. Andrews, D. V. Gorelov, C. Huang, D. Kim, T. J. T. Kwan, K. Nichols, J. W. I. Lewellen, V. Pavlenko, J. Shao, J. Power, S. Antipov, C. Jing, S. Lewis and E. Nanni. High current field emission electron sources for linear colliders and RF source applications. Presented at *Snowmass 21: Targets and Sources Kickoff meeting*, Batavia, Illinois, United States, 2020-09-28 - 2020-09-28. (LA-UR-20-28350)

Posters

Andrews, H. L., K. Nichols and E. I. Simakov. Novel Field-Emission Cathodes for National Security Accelerators. . (LA-UR-20-26767)

Kim, D., R. L. Fleming, H. L. Andrews, B. K. Choi, D. V. Gorelov, C. Huang, T. J. T. Kwan, J. W. I. Lewellen, K. Nichols, V. Pavlenko and E. I. Simakov. Divergence Study and Emittance Measurement for the Electron Beam Emitted from a Diamond Pyramid. Presented at *AAC 2020 Seminar*, Berkeley, California, United States, 2020-11-18 - 2020-11-18. (LA-UR-20-29588)

Nichols, K., D. Shchegolkov, E. I. Simakov and H. L. Andrews. MODELING OF DIAMOND FIELD EMITTER ARRAYS FOR SHAPED ELECTRON BEAM PRODUCTION. Presented at *IPAC*, Vancouver, Canada, 2018-04-29 - 2018-05-04. (LA-UR-18-23589)

Pavlenko, V., H. L. Andrews, R. L. Fleming, D. V. Gorelov, D. Kim and E. I. Simakov. Strong Field Photoemission Experiment using Diamond Field Emitter Arrays. Presented at *AAC 2020 Seminar*, Berkeley, California, United States, 2020-11-18 - 2020-11-18. (LA-UR-20-29586)

Schneider, M. E., D. Kim, K. Nichols, H. L. Andrews, E. I. Simakov, E. Jevarjian, S. Baryshev and J. Shao. Application of FEgen for Guided Development of Transversely Shaped Beams using Field Emission Arrays. Presented at *AAC Seminar Series 2020*, Virtual, California, United States, 2020-11-18 - 2021-01-06. (LA-UR-20-29454)

Schneider, M. E., E. Jevarjian, J. Shao, T. Posos, T. Nikhar, W. Lui and S. V. Baryshev. Developed and experimentally vetted ampere-class field emission cathode (FEC) operated up to 100 MV/m and Beyond Child Langmuir. Presented at *ACC Seminar Series*, Digital, California, United States, 2020-11-18 - 2021-01-06. (LA-UR-20-29445)

Stiftel, J. G. Beam shaping for 'shoebox' accelerators. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-26792)

Other

Nichols, K. JVST B Special Topic Collection on Vacuum Nanoelectronics - Call for Papers Images. Audio/Visual. (LA-UR-21-23886)

Pinning Down the Neutrino-proton Process Importance in Heavy Element Production via Reaction Studies on Radioactive Nickel-56

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Project Description

The entire project effort, from radioactive sample production at the Isotope Production Facility to performing neutron-induced reactions at Los Alamos Neutron Science Center, can be only performed at Los Alamos National Laboratory in the US. The project results will extend to the study of nuclear reactions on radioactive samples, directly related to NNSA missions, including radiochemical detector analysis, device diagnostics, and other areas. Through this project we will improve our understanding of nuclear reaction mechanisms with mission relevance.

Technical Outcomes

To better understand heavy element productions in core-collapse supernovae, the team measured the radioactive nickel-56 56Ni (n,p) reaction and demonstrated the new work flow for: producing the 6-day half life 56Ni isotope, transporting to the Hotcell for chemical separation and thin film fabrication, and directly measuring (n,p) and (n,a) reaction cross sections on 56Ni and 59Ni in the neutron energy range of 0.5 -10 Mega electron-volt. for the first time.

Publications

Journal Articles

DiGiovine, B. J., L. Zavorka, D. J. Ballard, C. Eiroa Lledo, A. Georgiadou, S. A. Kuvin, H. Y. Lee, J. S. Marquis, M. J. Mocko, V. Mocko, C. Vermeulen and D. G. J. Votaw. Optimization of Neutron Beam Transport with the Development of an Advanced Collimation System at the LANSCE Facility. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-21-24564)

*Kim, H. I., H. Y. Lee, T. Kawano, A. Georgiadou, S. A. Kuvin, L. Zavorka and M. W. Herman. New evaluation on angular distributions and energy spectra for neutron-induced charged-particle measurements. 2020. *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. **963**: 163699. (LA-UR-19-28775 DOI: 10.1016/j.nima.2020.163699)

Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, A. Georgiadou, S. M. Mosby, D. G. J. Votaw, M. C. White and L. Zavorka. Validation of neutron induced reactions on natural carbon using an active target at neutron energies up to 22 MeV at LANSCE. Submitted to *Physical Review C*. (LA-UR-21-23241)

Kuvin, S. A., H. Y. Lee, E. R. Birnbaum, B. J. DiGiovine, C. Eiroa Lledo, A. Georgiadou, M. W. Herman, T. Kawano, V. Mocko, S. M. Mosby, C. Vermeulen, D. G. J. Votaw, L. Zavorka, G. Perdikakis, P. Tsintari and H. Kim. Tests of statistical Hauser-Feshbach calculations on unstable nuclei via the direct measurement of $^{59}Ni(n,p)^{59}Co$ and $^{59}Ni(n,\alpha)^{56}Fe$ at neutron energies from 500 keV to 10 MeV at LANSCE. Submitted to *Physical Review C*. (LA-UR-21-25101)

Kuvin, S. A., H. Y. Lee, T. Kawano, B. J. DiGiovine, A. Georgiadou, C. Vermeulen, M. C. White, L. Zavorka and H. I. Kim. Non-statistical fluctuations in the $^{35}Cl(n,p)^{35}S$ reaction cross section at fast neutron energies. Submitted to *Physical Review C*. (LA-UR-20-22546)

Lee, H. Y., S. M. Mosby, C. J. Prokop, A. M. Long, J. Goerres, E. Stech and M. Wiescher. Low Energy Neutron-induced Charged-particle (Z) (LENZ) instrument development with a focus on the Pulse Shape Discrimination for double-sided silicon strip detectors at LANSCE. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-19-29340)

Reports

DiGiovine, B. J. WNR Facility T4GEN2 Spallation Target Upgrade. Unpublished report. (LA-UR-20-30500)

DiGiovine, B. J. and L. Zavorka. WNR Facility Flight Path 90L Advanced Collimation Development. Unpublished report. (LA-UR-21-20779)

Lee, H. Y. Pinning Down the nu-p Process Importance in Heavy Element Production via Reaction Studies on Radioactive 56Ni at LANSCE. Unpublished report. (LA-UR-17-30772)

Lee, H. Y. LDRD Data Sheet for "Pinning Down the nu-p Process Importance in Heavy Element Production via Reaction Studies on Radioactive Ni-56 at LANSCE". Unpublished report. (LA-UR-18-25488)

Presentation Slides

Birnbaum, E. R. and C. Vermeulen. Isotope Production Facility Capabilities and Nuclear Physics Targetry. Presented at *LANSCE User Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30446)

DiGiovine, B. J. Enabling direct reaction studies with small, highly radioactive samples. Presented at *Workshop for Applied Nuclear Data Activities 2022*, Cisco WebEx (Virtually), New Mexico, United States, 2022-02-28 - 2022-02-04. (LA-UR-22-21560)

Grinder, M. M. and H. Y. Lee. Diamond Detectors in High Radiation Background. Presented at *NSSC-LANL Keepin Program presentation*, Los Alamos, New Mexico, United States, 2018-08-08 - 2018-08-08. (LA-UR-18-27519)

Kelly, K. J., H. Y. Lee, B. J. DiGiovine, S. A. Kuvin, L. Zavorka and A. Georgiadou. LANL experimental updates in FY19 on ChiNu and LENZ. Presented at *US Nuclear Data Week*, Brookhaven, New York, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31268)

Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, A. Georgiadou, L. Zavorka and H. I. Kim. Measurement of 35Cl(n,p)35S at LANSCE. Presented at *CSEWG*, Brookhaven, New York, United States, 2019-11-04 - 2019-11-06. (LA-UR-19-31100)

Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, C. Eiroa Lledo, A. Georgiadou, M. W. Herman, T. Kawano, H. I. Kim, S. A. Kozimor, V. Mocko, S. M. Mosby, E. M. O'Brien, C. Vermeulen, D. G. J. Votaw, L. Zavorka, G. Perdikakis and P. Tsintari. Study of 59Ni(n,p)59Co and 59Ni(n,a)56Fe at fast neutron energies. Presented at *CSEWG Nuclear Data Week*, Virtual, New York, United States, 2021-11-18 - 2021-11-18. (LA-UR-21-32061)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, S. M. Mosby, F. M. Nortier, C. Vermeulen, P. Tsintari, G. Perdikakis and M. M. Grinder. Constraining the \xce\xbdp-process through the study of neutron-induced charged-particle reactions on short-lived 56Ni. Presented at *APS April Meeting*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23602)

Kuvin, S. A., H. Y. Lee, T. Kawano, B. J. DiGiovine, A. Georgiadou, C. Vermeulen, M. C. White, D. G. J. Votaw, L. Zavorka and H. I. Kim. Neutron-induced charged-particle reaction studies at LANSCE and the first direct measurement of the 56Ni(n,p)56Co reaction.. Presented at *Virtual Seminar at UMass Lowell*, Lowell, Massachusetts, United States, 2021-04-02 - 2021-04-02. (LA-UR-21-23244)

Kuvin, S. A., H. Y. Lee, T. Kawano, B. J. DiGiovine, A. Georgiadou, C. Vermeulen, M. C. White, L. Zavorka and H. I. Kim. Nonstatistical fluctuations in the 35Cl(n, p)35S reaction cross section at fast-neutron energies. Presented at *Low Energy Community Meeting 2020*, Chicago, Illinois, United States, 2020-08-11 - 2020-08-12. (LA-UR-20-26109)

Kuvin, S. A., H. Y. Lee, T. Kawano, B. J. DiGiovine, A. Georgiadou, C. Vermeulen, M. C. White, L. Zavorka and H. I. Kim. Nonstatistical fluctuations in the 35Cl(n, p)35S reaction cross section at fast-neutron energies. Presented at *CSEWG 2020*, Virtual, New York, United States, 2020-12-02 - 2020-12-02. (LA-UR-20-29976)

Lee, H. Y., B. J. DiGiovine, L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, E. R. Birnbaum, M. Brugh, S. A. Kozimor, V. Mocko, F. M. Nortier, H. I. Kim, G. Perdikakis, P. Tsintari, C. Frohlich and M. Grinder. LENZ at LANSCE: neutron-induced charged-particle reaction studies on radioactive nuclei. Presented at *CENTAUR Scientific Advisory Committee Meeting*, Los Alamos, New Mexico, United States, 2019-08-21 - 2019-08-23. (LA-UR-19-28495)

Lee, H. Y., B. J. DiGiovine, L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, E. R. Birnbaum, M. Brugh, S. A. Kozimor and V. Mocko. LENZ at LANSCE: neutron-induced charged-particle reaction studies on radioactive nuclei. Presented at *Nuclear Data Workshop*, Livermore, California, United States, 2019-09-09 - 2019-09-13. (LA-UR-19-28969)

Lee, H. Y., L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman and H. I. Kim. New Evaluation on Angular Distributions and Energy Spectra for Neutron-induced Charged particle Measurements. Presented at *US Nuclear Data Program (CSEWG) meeting*, Brookhaven, New York, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31269)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, D. G. J. Votaw, L. Zavorka, C. Vermeulen, C. Eiroa Lledo, V. Mocko, E. R. Birnbaum, G. Perdikakis, P. Tsintari, C. Frohlich and T. Kawano. Direct measurement on radioactive 56,59Ni(n,p) reactions at Los Alamos Neutron Science Center (LANSCE). Presented at *The Institute of Nuclear and Particle Physics Seminar at Ohio University*, Athens, Ohio, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-29835)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, D. G. J. Votaw, L. Zavorka, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, V. Mocko, E. R. Birnbaum, G. Perdikakis, P. Tsintari and C. Frohlich. Direct measurement of neutron-induced reactions with radioactive 56,59Ni at Los Alamos Neutron Science Center (LANSCE). Presented at *2021 SSAP Symposium Stewardship Science Academic Programs Annual Review*, washington DC, District Of Columbia, United States, 2021-02-16 - 2021-02-18. (LA-UR-21-21448)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, D. G. J. Votaw, L. Zavorka, T. Kawano, M. W. Herman and P. E. Koehler. LANL experimental updates on LENZ and DICER in FY20. Presented at *US NDP Nuclear Data Week*,

Brookhaven, New York, United States, 2020-11-30 - 2020-12-04. (LA-UR-20-29936)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, L. Zavorka, G. M. Hale, T. Kawano, M. W. Paris, C. Vermeulen, C. Eiroa Lledo, V. Mocko, E. R. Birnbaum, G. Perdikakis, P. Tsintari and C. Frohlich. Improving predictions of nuclear reaction cross sections via precision measurements at Los Alamos Neutron Science Center (LANSCE). Presented at *University of Notre Dame, Nuclear Physics Seminar*, Notre Dame, Indiana, United States, 2020-02-03 - 2020-02-03. (LA-UR-20-21014)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, P. E. Koehler, C. Vermeulen, C. Eiroa Lledo, V. Mocko, E. R. Birnbaum, G. Perdikakis and P. Tsintari. Radioactive target needs for nuclear data. Presented at *Workshop for Applied Nuclear Data Activities (WANDA)*, Washington DC, District Of Columbia, United States, 2020-03-03 - 2020-03-06. (LA-UR-20-22117)

Lee, H. Y., S. A. Kuvin, L. Zavorka, T. Kawano, C. Vermeulen, K. Bennett, E. R. Birnbaum, M. Brugh, F. M. Nortier, G. Perdikakis, P. Tsintari, M. Grinder and C. Frohlich. First Direct Measurement on 56Ni(n,p) Reaction for Astrophysical Implication. Presented at *The Fall Meeting of Division of Nuclear Physics of the American Physical Society*, Waikoloa village, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30291)

Tsintari, P., G. Perdikakis, P. Gastis, J. Dissanayake, J. Davison, Z. Purcell, H. Y. Lee, S. A. Kuvin, L. Zavorka, A. Georgiadou and H. Kim. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *Frontiers Junior Researchers Workshop*, East Lancing, Michigan, United States, 2019-05-20 - 2019-05-21. (LA-UR-19-24752)

Tsintari, P., G. Perdikaks, J. Dissanayake, J. Davison, Z. Purcell, H. Y. Lee, S. A. Kuvin, L. Zavorka, A. Georgiadou and H. I. Kim. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *WE-Heraeus summer school on Nuclear Physics in Astrophysics*, Heidelberg, Germany, 2019-09-10 - 2019-09-14. (LA-UR-19-29020)

Vermeulen, C., H. Y. Lee, E. R. Birnbaum, F. M. Nortier, S. A. Kuvin, K. Bennett and G. Pederkakis. Radioactive Targets at Los Alamos National Laboratory: A quasi-philosophical approach. Presented at *25th Conference on Application of Accelerators in Research and Industry*, Grapevine, Texas, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27361)

Posters

Grinder, M., H. Iwasaki, T. Mijatovic, R. Elder, J. Ash, A. Revel, H. Y. Lee and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Implementation of a Radiation-hard Diamond Active Target. Presented at *NSSC University Program Review 2019*, Releigh, North Carolina, United States, 2019-06-04 - 2019-06-06. (LA-UR-19-24418)

Grinder, M., H. Iwasaki, T. Mijatovic, R. Elder, J. Ash, H. Y. Lee and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Diamond Detectors in High Radiation Background. Presented at *The Nuclear Science and Security Consortium Fall Workshop*, Livermore, California, United States, 2018-10-01 - 2018-10-02. (LA-UR-18-29099)

Grinder, M., H. Y. Lee, H. Iwasaki, T. Mijatovic, R. Elder, J. Ash and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Implementation of a Radiation-Hard Active Target. Presented at *NSSC University Program Review 2018*, Ann Arbor, Michigan, United States, 2018-06-05 - 2018-06-07. (LA-UR-18-23629)

Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, C. Vermeulen and C. Eiroa Lledo. Measurement of the\xc2\xa059Ni(n,p) reaction at LANSCE and progress towards the first direct measurement of the 56Ni(n,p) reaction. Presented at *agnew showcase*, los alamos, New Mexico, United States, 2019-12-10 - 2019-12-10. (LA-UR-19-32221)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, M. Grinder, S. M. Mosby, F. M. Nortier, G. Perdikakis, P. Tsintari and C. Vermeulen. Constraining the nu p-process through the study of neutron-induced charged-particle reactions on short-lived 56Ni. Presented at *Conference on Compound Nuclear Reactions*, Berkeley, California, United States, 2018-09-24 - 2018-09-28. (LA-UR-18-29018)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, M. Grinder, S. M. Mosby, F. M. Nortier, G. Perdikakis, P. Tsintari and C. Vermeulen. First Direct Measurement of the 56Ni(n,p) Reaction. Presented at *LANSCE User Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-07. (LA-UR-18-30461)

Kuvin, S. A. and L. Collaboration. Progress towards the first direct measurement of the 56Ni(n,p) reaction. Presented at *Gordon Research Conference*, New London, New Hampshire, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25358)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, A. Georgiadou, D. G. J. Votaw, T. Kawano, M. W. Herman and H. I. Kim. High precision neutron-induced charged particle reaction study using Low Energy NZ (LENZ). . (LA-UR-21-28955)

Lee, H. Y., S. A. Kuvin, B. J. DiGiovine, S. M. Mosby, D. G. J. Votaw, C. Vermeulen, E. R. Birnbaum and V. Mocko. Unique capability to directly study nuclear reactions on short-lived radionuclide at LANSCE. . (LA-UR-21-28957)

Tsintari, P., G. Perdikakis, J. Davison, Z. Purcell, H. Y. Lee, L. Zavorka and C. Frohlich. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *WE-Heraeus summer school on Nuclear Physics in Astrophysics*, Heidelberg, Germany, 2019-09-10 - 2019-09-14. (LA-UR-19-29021)

Tsintari, P., G. Perdikakis, J. Davison, Z. Purcell and H. Y. Lee. Optimization of the LENZ detector system at LANL for the study of (n,p) reactions with radioactive targets using GEANT4 simulations. . (LA-UR-18-29098)

Ultra-Diffuse Galaxies, Tidal Streams and Dwarf Galaxies: The Low-Surface Brightness Frontier

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Project Description

Detecting low surface brightness features is a long standing challenge for optical imagers that are conducting national security missions. The new imaging technology and image software that we are developing will dramatically improve the ability to detect low surface brightness features that would otherwise has gone undetected. Successful development of technology has the potential to favorably impact our capability to conduct the DOE/NNSA treaty monitoring mission. Additionally, it is likely to have important application to difficult remote sensing problems like the detection of plumes and chemical release clouds.

Technical Outcomes

This project successfully established a new capability to detect diffuse, very low surface brightness, sources in the night sky. A hybrid telescope array was built that, for the first time, combines coarse and fine resolution imagers to increase the sensitivity to diffuse extended features while mitigating potential false positives generated by point source confusion. The team developed software that enables the construction of sensitive image stacks for application to astronomical research and Space Domain Awareness.

Publications

Journal Articles

*Bellm, E. C., S. R. Kulkarni, M. J. Graham, R. Dekany, R. M. Smith, R. Riddle, F. J. Masci, G. Helou, T. A. Prince, S. M. Adams, C. Barbarino, T. Barlow, J. Bauer, R. Beck, J. Belicki, R. Biswas, N. Blagorodnova, D. Bodewits, B. Bolin, V. Brinnel, T. Brooke, B. Bue, M. Bulla, R. Burruss, S. B. Cenko, C. Chang, A. Connolly, M. Coughlin, J. Cromer, V. Cunningham, K. De, A. Delacroix, V. Desai, D. A. Duev, G. Eadie, T. L. Farnham, M. Feeney, U. Feindt, D. Flynn, A. Franckowiak, S. Frederick, C. Fremling, A. Gal-Yam, S. Gezari, M. Giomi, D. A. Goldstein, V. Z. Golkhou, A. Goobar, S. Groom, E. Hacopians, D. Hale, J. Henning, A. Y. Q. Ho, D. Hover, J. Howell, T. Hung, D. Huppenkothen, D. Imel, W. Ip, Z. Ivezic, E. Jackson, L. Jones, M. Juric, M. M. Kasliwal, S. Kaspi, S. Kaye, M. S. P. Kelley, M. Kowalski, E. Kramer, T. Kupfer, W. Landry, R. R. Laher, C. Lee, H. W. Lin, Z. Lin, R. Lunnan, M. Giomi, A. Mahabal, P. Mao, A. A. Miller, S. Monkewitz, P. Murphy, C. Ngeow, J. Nordin, P. Nugent, E. Ofek, M. T. Patterson, B. Penprase, M. Porter, L. Rauch, U. Rebbapragada, D. Reiley, M. Rigault, H. Rodriguez, J. van Roestel, B. Rusholme, J. van Santen, S. Schulze, D. L. Shupe, L. P. Singer, M. T. Soumagnac, R. Stein, J. Surace, J. Sollerman, P. Szkody, F. Taddia, S. Terek, A. Van Sistine, S. van Velzen, W. T. Vestrand, R. Walters, C. Ward, Q. Ye, P. Yu, L. Yan and J. Zolkower. The Zwicky Transient Facility: System Overview, Performance, and First Results. 2019. *Publications of the Astronomical Society of the Pacific*. **131** (995): 018002. (LA-UR-19-22558 DOI: 10.1088/1538-3873/aaecbe)

*Graham, M. J., S. R. Kulkarni, E. C. Bellm, S. M. Adams, C. Barbarino, N. Blagorodnova, D. Bodewits, B. Bolin, P. R. Brady, S. B. Cenko, C. Chang, M. W. Coughlin, K. De, G. Eadie, T. L. Farnham, U. Feindt, A. Franckowiak, C. Fremling, S. Gezari, S. Ghosh, D. A. Goldstein, V. Z. Golkhou, A. Goobar, A. Y. Q. Ho, D. Huppenkothen, Z. Ivezic, R. L. Jones, M. Juric, D. L. Kaplan, M. M. Kasliwal, M. S. P. Kelley, T. Kupfer, C. Lee, H. W. Lin, R. Lunnan, A. A. Mahabal, A. A. Miller, C. Ngeow, P. Nugent, E. O. Ofek, T. A. Prince, L. Rauch, J. van Roestel, S. Schulze, L. P. Singer, J. Sollerman, F. Taddia, L. Yan, Q. Ye, P. Yu, T. Barlow, J. Bauer, R. Beck, J. Belicki, R. Biswas, V. Brinnel, T. Brooke, B. Bue, M. Bulla, R. Burruss, A. Connolly, J. Cromer, V. Cunningham, R. Dekany, A. Delacroix, V. Desai, D. A. Duev, M. Feeney, D. Flynn, S. Frederick, A. Gal-Yam, M. Giomi, S. Groom, E. Hacopians, D. Hale, G. Helou, J. Henning, D. Hover, L. A. Hillenbrand, J. Howell, T. Hung, D. Imel, W. Ip, E. Jackson, S. Kaspi, S. Kaye, M. Kowalski, E. Kramer, M. Kuhn, W. Landry, R. R. Laher, P. Mao, F. J. Masci, S. Monkewitz, P. Murphy, J. Nordin, M. T. Patterson, B. Penprase, M. Porter, U. Rebbapragada, D. Reiley, R. Riddle, M. Rigault, H. Rodriguez, B. Rusholme, J. van Santen, D. L. Shupe, R. M. Smith, M. T. Soumagnac, R. Stein, J. Surace, P. Szkody, S. Terek, A. Van Sistine, S. van Velzen, W. T. Vestrand, R. Walters, C. Ward, C. Zhang and J. Zolkower. The Zwicky Transient Facility: Science Objectives. 2019. *Publications of the Astronomical Society of the Pacific*. **131** (1001): 078001. (LA-UR-19-30653 DOI: 10.1088/1538-3873/ab006c)

*Panaitescu, A. X-Ray Afterglows from the Gamma-Ray Burst "Large-angle" Emission. 2020. *The Astrophysical Journal*. **895** (1): 39. (LA-UR-20-21724 DOI: 10.3847/1538-4357/ab8bdf)

Vestrand, W. T., P. F. Bloser, A. S. Hoover, L. P. Parker and J. Wren. The Mini Astrophysical MeV Background Observatory (MAMBO): A CubeSat for measuring the MeV Extragalactic Gamma-Ray Background. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-26775)

Vestrand, W. T. and L. P. Parker. Optical Emission from Fossil Cosmic Ray Reservoirs. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-27021)

Conference Papers

Parker, L. P., Y. H. Sechrest, W. T. Vestrand, P. R. Wozniak and D. Palmer. A Heterogeneous Telescope Array Optimized For Low Surface Brightness Imaging. Presented at *SPIE Astronomical Telescopes + Instrumentation (digital, remote)*. (Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16). (LA-UR-20-29825)

Presentation Slides

Parker, L. P. A Heterogeneous Telescope Array Optimized For Low Surface Brightness Imaging. Presented at *SPIE Astonomical Telescopes + Instrumentation (digital, remote)*, Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-29819)

Posters

Parker, L. P. A Heterogeneous Telescope Array Optimized For Low Surface Brightness Imaging. Presented at *SPIE Astronomical Telescopes + Instrumentation (digital, remote conference)*, Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-29826)

Using Quarkonia to Probe Matter from the Early Universe

Ivan Vitev
20190033ER

Project Description

A millionth of a second after the Big Bang, while still at a temperature of several trillion degrees, the entire universe transitioned through a phase of matter we are only beginning to understand--- the quark-gluon plasma (QGP), a hot and dense soup of the most fundamental microscopic constituents that make up the visible world. As this strongly interacting plasma expanded and cooled down, quarks and gluons clumped together into bound states to form a gas of particles called hadrons. This phase transition is of great interest to particle and nuclear physics, cosmology and astrophysics. It was predicted to affect the density of dark matter, and result in gravitational waves that probe the QGP properties. Heavy ion physics is a forefront area of research at the interface of high-energy and nuclear science that seeks to recreate these primordial states of matter of the early universe in controlled laboratory conditions and pin down their properties by colliding nuclei at ultrarelativistic energies. We will develop a new theory that describes some of the heaviest elementary particles produced in nature, called quarkonia, and use them to determine the properties of a primordial state of matter created in heavy ion collisions and the early universe.

Technical Outcomes

The technical advances that this project enabled are critical for the understanding of heavy flavor and quarkonium production. The team's research resulted into significantly improved description of the charmonium and bottomonium suppression in heavy ion collisions. It provided the broader community with novel theoretical tools and allowed for independent extraction of the temperature and transport properties of the quark-gluon plasma. The project was a success and positioned Los Alamos as a leader in the field.

Publications

Journal Articles

Fleming, S., Y. Makris and T. Mehen. An effective field theory approach to quarkonium at small transverse momentum. Submitted to *Journal of High Energy Physics*. (LA-UR-19-31110)

*Gao, A., H. T. Li, I. Moult and H. X. Zhu. Precision QCD Event Shapes at Hadron Colliders: The Transverse Energy-Energy Correlator in the Back-to-Back Limit. 2019. *Physical Review Letters*. **123** (6): 062001. (LA-UR-19-20914 DOI: 10.1103/PhysRevLett.123.062001)

Gutierrez-Reyes, D., Y. Makris, V. P. Vaidya, I. Scimemi and L. Zoppi. Probing Transverse-Momentum Distributions With Groomed Jets. Submitted to *Journal of High Energy Physics*. (LA-UR-19-31102)

*Kang, Z., J. Reiten, I. Vitev and B. Yoon. Light and heavy flavor dijet production and dijet mass modification in heavy ion collisions. 2019. *Physical Review D*. **99** (3): 034006. (LA-UR-19-22344 DOI: 10.1103/PhysRevD.99.034006)

*Lee, C., P. Shrivastava and V. Vaidya. Predictions for energy correlators probing substructure of groomed heavy quark jets. 2019. *Journal of High Energy Physics*. **2019** (9): 45. (LA-UR-18-24853 DOI: 10.1007/JHEP09(2019)045)

*Li, C. S., H. T. Li, D. Y. Shao and J. Wang. Momentum-space threshold resummation in tW production at the LHC. 2019. *Journal of High Energy Physics*. **2019** (6): 125. (LA-UR-19-21475 DOI: 10.1007/JHEP06(2019)125)

Li, H. T. and I. Vitev. Jet splitting function in the vacuum and QCD medium. *PoS - Proceedings of Science*. (LA-UR-19-20679 DOI: 10.22323/1.345.0077)

*Li, H. T. and I. Vitev. Inclusive heavy flavor jet production with semi-inclusive jet functions: from proton to heavy-ion collisions. 2019. *Journal of High Energy Physics*. **2019** (7): 148. (LA-UR-19-20952 DOI: 10.1007/JHEP07(2019)148)

Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in h \xe2\x86\x92\xce\xb3\xce\xb3 Decay: II. Renormalization and Scale Evolution. Submitted to *Journal of High Energy Physics*. (LA-UR-20-28938)

Makris, Y. Mitigating large background using subtracted jet substructure moments. Submitted to *Physical Review D*. (LA-UR-18-31092)

Makris, Y. and I. M. Vitev. An Effective Theory of Quarkonia in QCD Matter. Submitted to *Journal of High Energy Physics*. (LA-UR-19-25833)

*Sievert, M. D., I. Vitev and B. Yoon. A complete set of in-medium splitting functions to any order in opacity. 2019. *Physics Letters B*. **795**: 502-510. (LA-UR-19-22343 DOI: 10.1016/j.physletb.2019.06.019)

Vitev, I. Aspects of heavy flavor jet physics in heavy ion collisions. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30718 DOI: 10.22323/1.355.0009)

Vitev, I. Toward an effective theory of quarkonium production nuclear matter. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30716 DOI: 10.22323/1.355.0041)

Vitev, I. M., A. Sadofyev and M. Sievert. Ab Initio Coupling of Jets to Collective Flow in the Opacity Expansion Approach. Submitted to *Journal of High Energy Physics*. (LA-UR-21-21420)

Vitev, I. M., H. Li and Z. Liu. Heavy meson tomography of cold nuclear matter at the electron-ion collider. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-20-28004)

Vitev, I. M. and J. Lansberg. Perspectives for quarkonium studies at high-luminosity LHC. Submitted to *Elsevier journal family*. (LA-UR-20-28018)

Vitev, I. M. and Y. Makris. An Effective Theory of Quarkonia in QCD Matter. Submitted to *Nuclear Physics A*. (LA-UR-20-28019)

Books/Chapters

Lee, C., I. M. Vitev, R. Boussarie, J. W. Qiu, I. W. Stewart, T. Mehen, M. Burkardt, M. Constantinou, W. Detmold, M. Ebert, M. Engelhardt, S. Fleming, L. Gamberg, X. Ji, Z. B. Kang, K. F. Liu, S. Liuti, A. Metz, J. Negele, D. Pitonyak, A. Prokudin, A. Rajan, M. Schlegel, P. Shanahan, P. Schweitzer, A. Tarasov, R. Venugopalan, F. Yuan and Y. Zhao. TMD Handbook: A modern introduction to the physics of Transverse Momentum Dependent distributions. (LA-UR-21-20798)

Da Silva, C. L., J. M. Durham, C. Lee, X. Li, M. X. Liu, A. Morreale, W. E. Sondheim, I. M. Vitev, B. Surrow, R. Milner, A. Dumitru, O. Evdomikov, A. Metz, C. Muñoz Camacho, K. Barish, T. Horn, P. Jones, S. Dalla Torre, M. Diefenthaler and C. Wong. EIC Yellow Report. (LA-UR-21-20953)

Reports

Vitev, I. M. Future physics opportunities for high-density QCD at the LHC with heavy-ion and proton beam. Unpublished report. (LA-UR-19-22345)

Presentation Slides

Lee, C., B. Yan, B. Yoon, G. Bell, Y. Makris and J. Talbert. Angularities, gaps, and \\alpha_s. Presented at *World SCET 2021*, Cambridge, Massachusetts, United States, 2021-04-19 - 2021-04-23. (LA-UR-21-23742)

Lee, C., B. Yoon, B. Yan, Y. Makris, J. Talbert and G. Bell. Event shape tails and alpha_s. Presented at *INT Workshop on Probing QCD at High Energy and Density with Jets*, Seattle, Washington, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-27921)

Tomalak, O. S. QED radiative corrections to charged-current neutrino-nucleon elastic scattering for accelerator neutrino experiment. Presented at *NuFact 2021: The 22nd International Workshop on Neutrinos from Accelerators*, Cagliari, Italy, 2021-09-05 - 2021-09-11. (LA-UR-21-28076)

Tomalak, O. S. Axial and pseudoscalar form factors with tau neutrinos. Presented at *Tau Neutrinos from GeV to EeV 2021 (NuTau2021)*, Upton, New York, United States, 2021-09-28 - 2021-10-01. (LA-UR-21-28872)

Tomalak, O. S. QED radiative corrections to charged-current neutrino-nucleon elastic scattering for accelerator neutrino experiments. Presented at *FNAL Neutrino Joint Theory-Experiment Working Group Meeting*, Batavia, Illinois, United States, 2021-09-23 - 2021-09-23. (LA-UR-21-29212)

A New Computation Framework for the Nonlinear Beam Dynamics with Radiation Self-fields

Chengkun Huang
20190131ER

Project Description

The development of X-ray Free Electron Lasers (FELs) and compact advanced accelerators provides the foundation to address the control of performance and production of materials at the mesoscale, a major challenge in national security missions. The continuing quest to enhance the performance/functionality of X-ray FELs and advance accelerators demands techniques to manipulate electron beams with the highest brightness. However, nonlinear beam dynamic problems often arise in the generation and control of such beams. State-of-the-art theoretical and simulation models lack the accuracy and physics consistency to fully address these outstanding beam dynamic problems. We will design and implement a new simulation framework to treat the self-consistent dynamics of a relativistic particle beam interacting with its complete radiation self-fields. With the unprecedented accuracy and physics consistency, this tool will be applied to the evaluation of high risk component design in free electron lasers.

Technical Outcomes

A state-of-the-art exascale-ready simulation tool "CoSyR" has been developed for the understanding of synchrotron radiations and their effects on the beam dynamics, This tool employs a novel Lagrangian method using wavefront/wavelet meshes for the calculation of the particles' radiation near-fields via the Green's function of the Maxwell equations. Fully self-consistent simulations are carried out for the first time, which reveal a complex interplay between the longitudinal and transverse coherent fields by the beam.

Publications

Journal Articles

Huang, C., F. Li, H. N. Rakotoarivelo, B. Shen, J. Domine, B. E. Carlsten, G. A. Dilts, R. V. Garimella, T. J. T. Kwan and R. W. Robey. CoSyR: a novel beam dynamics code for the modeling of synchrotron radiation effects. Submitted to *Physical Review Special Topics in Accelerator and Beams*. (LA-UR-21-29084)

B. M. *. C. N. M. *. H. Y. *. H. G. *. H. A. *. H. C. *. L. M. H. *. M. C. E. *. M. C. E. *. N. C. *. Q. J. *. R. R. D. *. S. A. *. S. E. *. V. J. *. W. D. *. Z. H. Sagan, D. *., A. Scheinker and C. -. K. Huang. Simulations of future particle accelerators: issues and mitigations. 2021. *Journal of Instrumentation*. **16** (10): T10002. (LA-UR-21-27695 DOI: 10.1088/1748-0221/16/10/T10002)

Conference Papers

Li, F., C. Huang, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Validation of a novel method for the calculation of near-field synchrotron radiation. Presented at *10th International Particle Accelerator Conference*. (Melbourne, Australia, 2019-05-19 - 2019-05-24). (LA-UR-19-24377)

Reports

Gress, G. J. Understanding machine learning approaches for partial differential equations. Unpublished report. (LA-UR-20-27592)

Yeung, O. B. Validation of Two-Dimensional Near-Field Synchrotron Radiation Solver. Unpublished report. (LA-UR-19-27333)

Presentation Slides

Domine, J. Coherent Synchrotron Radiation (CoSyR): Optimizing the Memory-Bound Interpolation Module. Presented at *Parallel Computing Student Project Outbrief*, Los Alamos, New Mexico, United States, 2021-08-05 - 2021-08-05. (LA-UR-21-27800)

Huang, C. Particle accelerators: present, future and the enabling computational modeling. . (LA-UR-19-31915)

Huang, C., F. Li, H. N. Rakotoarivelo, B. Shen, R. V. Garimella, O. B. Yeung, P. P. Pombrio, T. J. T. Kwan and B. E. Carlsten. A Particle-Mesh Method for the Modeling of Synchrotron Radiation from Electron Beam. Presented at *47th IEEE International Conference On Plasma Sciences (virtual)*, online, New Mexico, United States, 2020-12-06 - 2020-12-10. (LA-UR-20-29999)

Huang, C., F. Li, H. N. Rakotoarivelo, O. B. Yeung, P. P. Pombrio, B. Shen, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. A Particle-Mesh Method for the Modeling of Synchrotron Radiation from Electron Beam. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, online, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29142)

Huang, C., F. Li, O. B. Yeung, P. P. Pombrio, B. Shen, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Comparison of Numerical Methods for the Calculation of Synchrotron Radiation from Electrons. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30731)

Li, F., C. Huang, O. B. Yeung, B. Shen, P. P. Pombrio, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Comparison of Numerical Methods for the Calculation of Synchrotron Radiation from Electrons. Presented at *North American Particle Accelerator Conference*, Lansing, Michigan, United States, 2019-09-01 - 2019-09-06. (LA-UR-19-28858)

Shen, B. Numerical Method and Parallelization for the Computation of Synchrotron Radiation. Presented at *Super Computing 2019*, Denver, Colorado, United States, 2019-11-17 - 2019-11-17. (LA-UR-19-27982)

Yeung, O. B. Design and Validation of a Solver for Synchrotron Radiation. Presented at *LANL SULI Presentations, on-site*, Los Alamos, New Mexico, United States, 2019-07-17 - 2019-07-17. (LA-UR-19-27178)

Posters

Huang, C., F. Li, H. N. Rakotoarivelo, B. E. Carlsten, T. J. T. Kwan, R. V. Garimella, G. A. Dilts and R. W. Robey. Self-consistent Modeling Of Coherent Synchrotron Radiation From Electron Beams In Bunch Compressors. Presented at *12th International Particle Accelerator Conference*, Campinas, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24969)

Li, F., C. Huang, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Validation of a novel method for the calculation of near-field synchrotron radiation. Presented at *10th International Particle Accelerator Conference*, Melbourne, Australia, 2019-05-19 - 2019-05-24. (LA-UR-19-24589)

Shen, B. Numerical Method and Parallelization for the Computation of Synchrotron Radiation. Presented at *Super Computing 19*, Denver, Colorado, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-27461)

Shen, B. Numerical Method for the Computation of Synchrotron Radiation in the Near-Field. Presented at *PCSRI Outbrief Presentations*, Los alamos, New Mexico, United States, 2019-07-30 - 2019-07-30. (LA-UR-19-27494)

The Influence of Multiple Scattering on the Opacities of Warm and Hot Dense Matter

Charles Starrett
20190206ER

Project Description

Opacity is a key quantity in weapons physics as well as inertial fusion and astrophysics. Our project will develop an new computational capability for opacity in dense plasmas -- a significant improvement over existing methods. The key advantage of our approach is that plasma effects will be fully accounted for in a non-perturbative way, in contrast to existing methods. We will apply this to open and enigmatic experiments that point to weaknesses in current approaches.

Technical Outcomes

The goal of assessing the impact of multiple scattering on opacity in warm and hot dense matter was successfully achieved. Another achievement was the successful use of the code for equation of state research.

Publications

Journal Articles

*F. C. *. S. C. Gill, N. *., N. M. Gill, C. J. Fontes and C. E. Starrett. Time-dependent density functional theory applied to average atom opacity. 2021. *Physical Review E*. **103** (4): 043206. (LA-UR-21-20133 DOI: 10.1103/PhysRevE.103.043206)

Shaffer, N. R. and C. E. Starrett. Multiple-Scattering Effect in Dense Plasma Opacity. Submitted to *Physical Review E*. (LA-UR-21-29199)

Starrett, C. E. and N. R. Shaffer. Multiple Scattering Theory for Dense Plasmas. Submitted to *Physical Review E*. (LA-UR-20-26583)

White, J. R., W. R. Johns, C. J. Fontes, N. M. Gill, N. R. Shaffer and C. E. Starrett. Charge State Distributions in Dense Plasmas. Submitted to *High Energy Density Physics*. (LA-UR-20-27503)

Reports

Abrams, J. R., B. W. Bell, T. S. Blade, J. W. Dyer, F. Holguin, J. S. Keithley, H. Leiendecker, W. R. Johns, E. C. Koskelo, N. Y.

Lo, O. G. Martin, A. P. May, T. M. Natan, L. V. Nguyen, C. F. Ottoway, D. A. Owens, S. D. Ozier, A. D. Somers, T. J. Taylor, A. J. Warhover, J. R. White, Q. M. White, C. J. Young, M. T. Andrews, G. R. Maskaly and D. M. Israel. Final Reports of the 2020 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-20-28407)

Alberse, J. R., A. E. Biewer, S. E. Campbell, H. S. Chalfin, C. A. J. Coffelt, D. K. Coffman, B. H. Fore, J. A. Freiberg, C. J. Hanson, S. Hegde, B. F. Hellwig, S. Joshi, C. R. Kumar, M. W. Laraia, J. T. Laune, L. L. Lin, C. X. Meng, A. M. Nemeth, C. S. Parker, D. M. Perez, S. Pineda, T. A. Saxton, T. Skaras, M. T. Andrews, D. M. Israel and G. R. Maskaly. Final Reports of the 2019 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-21-21581)

Gill, N. M. Modeling of Warm Dense Plasmas for the Determination of Transport Properties and Equation of State. Unpublished report. (LA-UR-20-22190)

Laraia, M. W., C. J. Hanson, N. R. Shaffer, D. Saumon, D. P. Kilcrease and C. E. Starrett. Real-Space Green's functions for Warm Dense Matter. Unpublished report. (LA-UR-20-30465)

Presentation Slides

Shaffer, N. R. and C. E. Starrett. Dense Plasma Opacity via Multiple Scattering Theory. Presented at *HED theory group meeting*, Rochester, New York, United States, 2021-03-11 - 2021-03-11. (LA-UR-21-22320)

Starrett, C. E. Electronic structure of Dense Plasma's with the Green's Function Method. . (LA-UR-19-29084)

Starrett, C. E. Towards a Complete and Consistent Model for Material Properties at Extreme Conditions. Presented at *NNSA ICF working group*, Remote, New Mexico, United States, 2020-12-16 - 2020-12-16. (LA-UR-20-30249)

Starrett, C. E. Superposition and Single Scattering: Missing Physics and Ionic Structure with an Average Atom Model. Presented at *Average Atom Models for Warm Dense Matter*, online, New Mexico, United States, 2021-06-28 - 2021-06-28. (LA-UR-21-25631)

Starrett, C. E. Multi-Center Calculations of the Equation of State at Very High Pressure. Presented at *APS DPP*, Pittsburg, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30357)

Starrett, C. E., D. Saumon and C. F. Ottoway. Equation of State of Aluminum and Carbon: An Evaluation Ionic Disorder in Plasma. Presented at *Materials/NLTE LDRD meeting*, Los Alamos, New Mexico, United States, 2021-05-17 - 2021-05-17. (LA-UR-21-24558)

Starrett, C. E., D. Saumon and C. F. Ottoway. Multi-Center Calculations of the Equation of State of Carbon at Very High Pressure. Presented at *PNP17*, Dresden, Germany, 2021-09-19 - 2021-09-19. (LA-UR-21-28884)

Starrett, C. E. and N. R. Shaffer. Multiple Scattering Theory for Dense Plasma Electronic Structure. . (LA-UR-20-27878)

Starrett, C. E. and N. R. Shaffer. Multiple Scattering Theory for Dense Plasma Electronic Structure. Presented at *APS March Meeting*, Online, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22323)

White, J. R., W. R. Johns, C. E. Starrett, N. R. Shaffer, C. J. Fontes and N. M. Gill. Photon Transport in Warm Dense Matter. . (LA-UR-20-26113)

Posters

Hanson, C. J., M. W. Laraia, C. E. Starrett, N. R. Shaffer and D. P. Kilcrease. Microfield distributions from pseudoatom molecular dynamics & Real-space structures for multiple scattering green's functions. . (LA-UR-19-27904)

Starrett, C. E. Using the Green's Function Multiple Scattering Method to Model Warm and Hot Dense Matter. Presented at *2019 Workshop on Recent Developments in Electronic Structure*, Urbana, Illinois, United States, 2019-05-19 - 2019-05-19. (LA-UR-19-24197)

A Non-Invasive Current Profile Diagnostic for Electron Bunches

Quinn Marksteiner
20190294ER

Project Description

This project will develop an electron beam diagnostic that will help resolve many important physics issues for high energy electron accelerators. This diagnostic will be of particular importance for accelerator capabilities, where a non-invasive diagnostic with short (femtosecond) resolution is needed to address important issues such as the microbunching instability and long-range wakes. In addition, the Department of Energy Office of Science Advanced Accelerator Development Strategy Report specifically calls out the need for diagnostics with femtosecond resolution, for laser-driven plasma wakefield accelerators and for particle-beam-driven plasma wakefield accelerators.

Technical Outcomes

The project was successful in building a diagnostic that is based on the measurement of off-axis undulator radiation. The diagnostic was built and sent to the Berkeley Lab Laser Accelerator (BELLA) for testing. The diagnostic included the undulator itself, along with associated optics, an Infared pyrometer that detects the signal, and software for looking at the data.

Publications

Journal Articles

Ostler, B. W., N. Yampolsky and Q. R. Marksteiner. Statistical analysis of electron bunch longitudinal profile reconstructions using the Gerchberg-Saxton algorithm. Submitted to *Review of Scientific Instruments*. (LA-UR-21-23366)

*Yampolsky, N., E. I. Simakov and A. Malyzhenkov. Imposing strong correlated energy spread on relativistic bunches with transverse deflecting cavities. 2020. *Physical Review Accelerators and Beams*. **23** (5): 054403. (LA-UR-19-30405 DOI: 10.1103/PhysRevAccelBeams.23.054403)

Presentation Slides

Marksteiner, Q. R., H. L. Andrews, S. Barber, J. E. Coleman, C. Emma, B. W. Ostler, W. P. Romero, R. Ryne and N. Yampolsky. Using off axis undulator radiation as a longitudinal current diagnostic. Presented at *Advanced Control Methods for Particle Accelerators*, Santa Fe, New Mexico, United States, 2019-08-20 - 2019-08-22. (LA-UR-19-28705)

Ostler, B. W. Developing a single-shot, nondestructive, and femtosecond resolution longitudinal charge density diagnostic for electron bunches; script. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25782)

Ostler, B. W., Q. R. Marksteiner, N. Yampolsky, H. L. Andrews, S. Barber, J. E. Coleman, C. Emma, W. P. Romero, R. D. Ryne, M. R. A. Zuboraj and J. van Tilborg. A High-Resolution and Noninvasive Longitudinal Profile Diagnostic for Electron Bunches. Presented at *Advanced Accelerator Concepts Seminar Series 2020 (Virtual)*, Los Alamos, New Mexico, United States, 2020-11-18 - 2021-02-03. (LA-UR-21-20100)

Ostler, B. W., Q. R. Marksteiner, N. Yampolsky, R. D. Ryne, R. L. Fleming, S. Barber, C. Emma and W. P. Romero. Developing a single-shot, nondestructive, and femtosecond resolution longitudinal charge density diagnostic for electron bunches. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25684)

Posters

Yampolsky, N., B. W. Ostler, C. Emma, H. L. Andrews, M. R. A. Zuboraj, Q. R. Marksteiner, S. Barber, F. Isono, R. D. Ryne and J. van Tilborg. Longitudinal diagnostics of ultra-short relativistic electron bunches based on coherent undulator radiation. Presented at *APS meeting, Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-07 - 2021-11-12. (LA-UR-21-31038)

Origin of High-Energy Astrophysical Neutrinos: Multi-messenger Signals from Flares of Extragalactic Jets

Hui Li
20190383ER

Project Description

This project aims at understanding the origin of high-energy astrophysical neutrinos, especially those made by relativistic jets powered by supermassive black holes. This is a fundamental question in our understanding of the cosmos. This project brings together theory, numerical modeling, observations in optical and gamma-rays. It builds capabilities in particle and gamma-ray detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Technical Outcomes

The theory team has developed the state-of-the-art simulation toolsets in simulations of relativistic particle acceleration processes. These capabilities place Los Alamos in a leadership position in modeling particle acceleration. The Los Alamos High-Altitude Water Cherenkov (HAWC) team was instrumental in developing the event reconstruction algorithms, which improve in sensitivity by a factor of 3-4. The team has determined that jets powered by supermassive black holes are indeed the most likely origin of high-energy astrophysical neutrinos.

Publications

Journal Articles

*Abeysekara, A. U., A. Albert, R. Alfaro, C. Alvarez, J. D. Alvarez, J. R. Angeles Camacho, R. Arceo, J. C. Arteaga-Velazquez, K. P. Arunbabu, D. Avila Rojas, H. A. A. Solares, V. Baghmanyan, E. Belmont-Moreno, S. Y. BenZvi, C. Brisbois, K. S. Caballero-Mora, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. Coutino de Leon, E. De la Fuente, C. de Leon, S. Dichiara, B. L. Dingus, M. A. DuVernois, J. C. Diaz-Velez, R. W. Ellsworth, K. Engel, C. Espinoza, B. Fick, H. Fleischhack, N. Fraija, A. Galvan-Gamez, J. A. Garcia-Gonzalez, F. Garfias, M. M. Gonzalez, J. A. Goodman, J. P. Harding, S. Hernandez, J. Hinton, B. Hona, F. Hueyotl-Zahuantitla, C. M. Hui, P. Huntemeyer, A. Iriarte, A. Jardin-Blicq, V. Joshi, S. Kaufmann, D. Kieda, A. Lara, W. H. Lee, H. Leon Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, J. Lundeen, K. Malone, S. S. Marinelli, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, H. Martinez-Huerta, J. A. Matthews, P. Miranda-Romagnoli, J. A. Morales-Soto, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, M. U. Nisa, R. Noriega-Papaqui, A. Peisker, E. G. Perez-Perez, J. Pretz, Z. Ren, C. D. Rho, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, E. Ruiz-Velasco, H. Salazar, F. S. Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, M. S. Arroyo, G. Sinnis, A. J. Smith, R. W. Springer, P. Surajbali, E. Tabachnick, M. Tanner, O. Tibolla, K. Tollefson, I. Torres, T. Weisgarber, S. Westerhoff, J. Wood, T. Yapici, A. Zepeda and H. Zhou. Measurement of the Crab Nebula Spectrum Past 100 TeV with HAWC. 2019. *The Astrophysical Journal*. **881** (2): 134. (LA-UR-19-24703 DOI: 10.3847/1538-4357/ab2f7d)

*Albert, A., R. Alfaro, D. Avila Rojas, V. Baghmanyan, E. Belmont-Moreno, C. Brisbois, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. Coutino de Leon, E. De la Fuente, C. de Leon, S. Dichiara, K. Engel, C. Espinoza, H. Fleischhack, N. Fraija, A. Galvan-Gamez, D. Garcia, F. Garfias, S. Hernandez, J. Hinton, B. Hona, D. Huang, F. Hueyotl-Zahuantitla, P. Huntemeyer, A. Iriarte, A. Jardin-Blicq, V. Joshi, S. Kaufmann, D. Kieda, A. Lara, H. Leon Vargas, G. Luis-Raya, J. Lundeen, R. Lopez-Coto, K. Malone, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, H. Martinez-Huerta, P. Miranda-Romagnoli, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, R. Noriega-Papaqui, A. Peisker, J. Pretz, Z. Ren, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, E. Ruiz-Velasco, F. S. Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, G. Sinnis, P. Surajbali, E. Tabachnick, M. Tanner, O. Tibolla, K. Tollefson, I. Torres, R. Torres-Escobedo, L. Villasenor, T. Weisgarber, J. Wood, T. Yapici, H. Zhang, H. Zhou, B. L. Dingus and J. P. Harding. Multiple Galactic Sources with Emission Above 56 TeV Detected by HAWC. 2020. *Physical Review Letters*. **124** (2): 021102. (LA-UR-19-29232 DOI: 10.1103/PhysRevLett.124.021102)

Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. Dahlin, Q. Zhang, J. Karpen and C. R. Devore. Slow Shock Formation Upstream of Reconnecting Current Sheets. Submitted to *Astrophysical Journal*. (LA-UR-21-27254)

Chen, Q., K. Nalewajko and B. P. Mishra. Scaling of Magnetic Dissipation and Particle Acceleration in ABC Fields. Submitted to *Journal of Plasma Physics*. (LA-UR-21-20632)

*Fowler, T. K., H. Li and R. Anantua. A Quasi-static Hyper-resistive Model of Ultra-high-energy Cosmic-ray Acceleration by Magnetically Collimated Jets Created by Active Galactic Nuclei. 2019. *The Astrophysical Journal*. **885** (1): 4. (LA-UR-20-28592 DOI: 10.3847/1538-4357/ab44bc)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

*Guo, F., X. Li, W. Daughton, P. Kilian, H. Li, Y. Liu, W. Yan and D. Ma. Determining the Dominant Acceleration Mechanism during Relativistic Magnetic Reconnection in Large-scale Systems. 2019. *Physical Review Letters*. **879** (2). (LA-UR-18-31752 DOI: 10.3847/2041-8213/ab2a15)

Guo, F., X. Li, W. S. Daughton, H. Li, P. F. H. Kilian, Y. H. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics and Particle Acceleration during Relativistic Turbulent Magnetic Reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-26005)

*Guo, F., Y. Liu, X. Li, H. Li, W. Daughton and P. Kilian. Recent progress on particle acceleration and reconnection physics during magnetic reconnection in the magnetically-dominated relativistic regime. 2020. *Physics of Plasmas*. **27** (8): 080501. (LA-UR-20-26135 DOI: 10.1063/5.0012094)

Hona, B., S. Casanova, K. Feng, P. Huentemeyer, A. Albert, M. Durocher, J. P. Harding and K. A. Malone. HAWC observations of the acceleration of very-high-energy cosmic rays in the Cygnus Cocoon. Submitted to *Nature Astronomy*. (LA-UR-21-22386)

*Kilian, P., X. Li, F. Guo and H. Li. Exploring the Acceleration Mechanisms for Particle Injection and Power-law Formation during Transrelativistic Magnetic Reconnection. 2020. *The Astrophysical Journal*. **899** (2): 151. (LA-UR-20-20135 DOI: 10.3847/1538-4357/aba1e9)

*Kong, X., F. Guo, Y. Chen and J. Giacalone. The Acceleration of Energetic Particles at Coronal Shocks and Emergence of a Double Power-law Feature in Particle Energy Spectra. 2019. *Astrophysical Journal*. **883** (1): 49. (LA-UR-19-20913 DOI: 10.3847/1538-4357/ab3848)

*Lazarian, A., G. L. Eyink, A. Jafari, G. Kowal, H. Li, S. Xu and E. T. Vishniac. 3D turbulent reconnection: Theory, tests, and astrophysical implications. 2020. *Physics of Plasmas*. **27** (1): 12305. (LA-UR-20-28591 DOI: 10.1063/1.5110603)

Lazarian, A., O. Khabarova, S. Xu and F. Guo. Violation of Flux Freezing, Turbulent Magnetic Reconnection and induced Particle Acceleration. Submitted to *Review of Modern Plasma Physics*. (LA-UR-21-27253)

Li, H. Fast Magnetic Reconnection with Turbulence in High Lundquist Number Limit. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-24765)

Li, H. 3D Numerical Simulation of Kink-driven Rayleigh–Taylor Instability Leading to Fast Magnetic Reconnection. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-28588)

Li, H. Energy occupation of waves and structures in 3D compressive MHD turbulence. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-28590)

*Loi, F., M. Murgia, F. Govoni, V. Vacca, A. Bonafede, C. Ferrari, I. Prandoni, L. Feretti, G. Giovannini and H. Li. Rotation measure synthesis applied to synthetic SKA images of galaxy clusters. 2019. *Monthly Notices of the Royal Astronomical Society*. **490** (4): 4841-4857. (LA-UR-20-28593 DOI: 10.1093/mnras/stz2699)

Malone, K. A., J. P. Harding, A. Albert, M. Durocher, S. Casanova, D. Huang, F. Salesa Greus, B. L. Dingus, G. J. Kunde, C. Brisbois and H. Zhou. Evidence of 200 TeV photons from HAWC J1825-134. Submitted to *Nature Astronomy*. (LA-UR-20-28703)

Malone, K. A. and B. L. Dingus. Multi-wavelength observations of 2HWC J1928+177: dark accelerator or new TeV gamma-ray binary?. Submitted to *Astrophysical Journal*. (LA-UR-20-28702)

Polko, P. and H. Li. Self-similar jet models: two new issues. Submitted to *Astrophysical Journal*. (LA-UR-19-30944)

Zhang, H., X. Li, D. Giannios, F. Guo, H. Thiersen, M. Bottcher, T. Lewis and T. Venters. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–II. Connection with gamma-rays. Submitted to *Astrophysical Journal*. (LA-UR-21-27252)

*Zhang, H., X. Li, D. Giannios, F. Guo, Y. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets. I. A Systematic Study. 2020. *The Astrophysical Journal*. **901** (2): 149. (LA-UR-20-20194 DOI: 10.3847/1538-4357/abb1b0)

Zhang, Q., F. Guo, W. S. Daughton, X. Li and H. Li. Efficient Nonthermal Ion and Electron Acceleration Enabled by the Flux-Rope KinkInstability in 3D Nonrelativistic Magnetic Reconnection. Submitted to *Physical Review Letters*. (LA-UR-21-24459)

Conference Papers

Dong, B., P. F. H. Kilian, X. Li, F. Guo, S. Byna and K. Wu. Terabyte-scale Particle Data Analysis: An ArrayUDF Case Study. Presented at *SSDBM 2019 : 31st International Conference on Scientific & Statistical Database Management*. (Santa Cruz, California, United States, 2019-07-23 - 2019-07-25). (LA-UR-19-24098)

Malone, K. A. Recent Results from the High Altitude Water Cherenkov Observatory. Presented at *International Symposium on Multiparticle Dynamics*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-13). (LA-UR-20-21318)

Reports

Rani, B., H. Zhang, S. Hunter, F. Kislat, M. Boettcher, J. E. McEnery, D. Giannios, F. Guo, H. Li, M. G. Baring, I. Agudo, S. Buson, M. Petropoulou, V. Pavlidou, E. Angelakis, I. Myserlis, Z. Wadiasingh, R. Curado da Silva, P. F. H. Kilian, S. Guiriec, V. Bozhilov, S. Anton, M. Kazana, P. Coppi, T. M. Venters, F. Longo and E. Bottachini. High-Energy Polarimetry - a new window to probe extreme physics in AGN jets. Unpublished report. (LA-UR-19-22708)

Presentation Slides

Guo, F. IC Project: Magnetic Reconnection versus Shocks: First-principles Kinetic Simulations of Major Particle Acceleration Mechanisms in the Universe. . (LA-UR-19-21782)

H. Kilian, P. F., X. Li, F. Guo and H. Li. How magnetic reconnection injects particles and accelerates them to high energies. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-22043)

H. Kilian, P. F. and F. Guo. Particle Acceleration due to Relativistic Reconnection. Presented at *235th AAS meeting*, Honolulu, Hawaii, United States, 2020-01-05 - 2020-01-08. (LA-UR-20-20084)

Li, H. All Hands On Deck: Understanding Astrophysical Jets. . (LA-UR-19-32437)

Li, H. Origin of High-Energy Astrophysical Neutrinos: Multi-Messenger Signals from Flares of Extra-galactic Jets. . (LA-UR-20-29526)

Li, H. IC Project: Production of High-Energy Cosmic Rays by Relativistic Magnetic Reconnection in Astrophysical Jets. . (LA-UR-21-23435)

Li, H. Instabilities and (Self-Generated) Turbulence and Implications for Particle Energization in Jets. Presented at *Extra-Galactic Jets at all scales*, Heidelberg, Germany, 2021-06-14 - 2021-06-14. (LA-UR-21-25651)

Malone, K. A. Observation of the highest-energy gamma rays with the HAWC Observatory. Presented at *P-3 seminar*, Virtual, New Mexico, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-22661)

Atomic Magnetometry for the neutron Electric Dipole Moment (nEDM) Experiment (Rosen Scholar)

Michael Furlanetto
20200003ER

Project Description

The research supported by this project addresses the question "Why does the Universe that we live in have so much more matter than antimatter", one of the biggest questions in present day science. This project, on completion, will have significantly contributed to demonstrating a capability to perform next generation experiments looking for neutron electric dipole moment, controlling systematics important for all such experiments. This research will have a profound impact on our understanding of the interaction among the fundamental building blocks of our world and the history of the Universe. The methods of precision measurements will benefit research performed at the Laboratory and elsewhere.

Technical Outcomes

Many important advancements were made in controlling and monitoring the magnetic field for the Los Alamos neutron Electric Dipole Moment (nEDM) experiment. Particularly of note is the completion of the field cage, a large coil structure. The field cage not only provided ways to improve the magnetic field stability and uniformity inside the Magnetically Shielded Room (MSR) by cancelling the ambient field but it also provided a tool to measure the performance of the MSR.

Advanced Fusion Concept for National Security Applications (U)

William Daughton
20200625ER

Project Description

The development of an experimental platform to study the physics of robustly burning plasmas has been a longstanding goal of the Department of Energy (DOE)/ National Nuclear Security Administration (NNSA). Such experiments would enable researchers to probe the nonlinear physics of thermonuclear burn and to further validate our simulation tools for stockpile stewardship activities.

Technical Outcomes

This project was successful in achieving the proposed objectives. Using several optimization strategies, our team developed designs that reached the specified goals in one-dimensional simulations. These designs were further evaluated within two-dimensional simulations and the results suggest a promising path forward. Working with experts across the laboratory, our team identified key physics and engineering uncertainties and devised appropriate experiments to address these issues.

An Alternative Approach to Inertial Confinement Fusion (ICF) Ignition and Burn Propagation at the National Ignition Facility (NIF)

Richard Olson
20200765ER

Project Description

The National Ignition Facility (NIF) is, by far, the largest laser facility in the world, and our nation has invested billions of dollars in its construction. Additional billions of dollars have been invested, so far, in the unsuccessful indirect drive Inertial Confinement Fusion (ICF) experiments using deuterium–tritium (DT) ice layer implosions. A new innovation to achieve ICF ignition and propagating burn using large Polar Direct Drive (PDD) capsules with liquid DT layers would be an important result for the national laboratories, the National Nuclear Security Administration (NNSA), and the nation. This project builds upon the work of the team responsible for nuclear survivability testing on NIF by not only Los Alamos National Laboratory (LANL), but also Lawrence Livermore National Laboratory (LLNL), Sandia National Laboratories (SNL), the Atomic Weapons Establishment (AWE), the United States Air Force, and the United States Navy. LANL's advanced engineering analysis and system design and analysis groups have been using the existing source for nuclear survivability testing of materials and system components. Achieving ICF ignition would garner world-wide recognition and usher in a new era of weapons-relevant experiments, including needs for studying mix and burn with an ignited plasma in addition to radiation effects testing needs.

Technical Outcomes

A new concept was developed for enhancing nuclear survivability testing capabilities for the National Nuclear Security Administration Laboratories, the US Air. Force, and the US Navy. Radiation-hydrodynamic code simulations indicate that this new concept can potentially increase neutron fluence by a factor of up to a thousand times the current testing capabilities at the National Ignition Facility.

Publications

Journal Articles

Olson, R. E., M. J. Schmitt, B. M. Haines, G. E. Kemp, C. B. Yeamans, B. E. Blue, D. W. Schmidt, A. Haid, M. Farrell, P. A. Bradley, H. F. I. Robey and R. J. Leeper. A polar direct drive liquid deuterium-tritium wetted foam target concept for inertial confinement fusion. Submitted to *Physics of Plasmas*. (LA-UR-21-25969)

Presentation Slides

Olson, R. E. Concept for increased neutron yield and potential ICF ignition at the NIF. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, on line, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28870)

Olson, R. E. A polar direct drive liquid deuterium-tritium wetted foam target concept for inertial confinement fusion. . (LA-UR-21-26170)

Olson, R. E. A polar direct drive liquid deuterium-tritium wetted foam inertial confinement fusion target concept. Presented at *LANL ICF-HED Update Meeting*, on line, New Mexico, United States, 2021-08-30 - 2021-08-30. (LA-UR-21-28476)

Olson, R. E., M. J. Schmitt, B. M. Haines, G. E. Kemp, C. Yeamans, B. Blue, D. W. Schmidt, A. Haid, M. Farrell, P. A. Bradley, H. F. I. Robey and R. J. Leeper. A polar direct drive liquid deuterium-tritium wetted foam inertial confinement fusion target concept. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30738)

Olson, R. E. and M. J. Schmitt. A polar direct drive liquid deuterium-tritium wetted foam inertial confinement fusion target concept. . (LA-UR-21-29451)

Neutron Experiment in Moon Orbit Pathfinder (NEMO 'Finder)

David Palmer
20210712ER

Project Description

NEMO 'Finder (Neutron Experiment in Moon Orbit Pathfinder) is a pair of spacecraft payloads that will space-qualify a new type of neutron detector and demonstrate a technique for finding the neutron lifetime, a quantity of both scientific and technical importance. In August 2020, Los Alamos National Laboratory (LANL) learned of an opportunity to place a scientific instrument on Cornell University's two spacecrafts that will orbit the Moon with the first National Aeronautics and Space Administration (NASA) Artemis launch. With unprecedented speed (10 weeks) LANL conceived, designed, constructed, tested, and prepared for delivery a pair of NEMO 'Finder payloads. We will now use the time before launch (scheduled Nov. 2021) to prepare to make use of the data that this mission will return. The results from the flight will allow new scientific and national security missions to proceed, both on Earth and in space.

Technical Outcomes

This project was highly successful in developing and demonstrating the use of a new type of sold-state neutron detector in a space-like environment. The technique for determining the neutron lifetime was also further developed. Although the originally-planned flight on Cornell's Cislunar Explorers has been delayed, the team pivoted and used this as an opportunity to fly the detectors on a series of high-altitude balloons to the Regener-Pfotzer Cosmic Ray Maximum.

Probabilistic Uncertainty Quantification Tools for Neutron Analysis

George McKenzie
20210715ER

Project Description

Tools to assess uncertainty are essential in all scientific work. A measurement without a confidence level does not allow scientists or key leaders to make fully-informed decisions. Neutron measurements validate nuclear data used to model all nuclear systems including: weapons, reactors, and nuclear processes required to manufacture things like pits. Neutron measurements are also used during nuclear incident response to perform a nuclear assessment and in particular give information on the system multiplication and mass. In both cases, an uncertainty would improve the quality of the measurement, and in the specific case of a nuclear incident response, this work will provide the first uncertainty quantification capability to better bound the nuclear assessment used by decision makers.

Technical Outcomes

This project set out to develop a tool to provide uncertainty quantification for neutron measurements. The final product of this work is a dynamic link library, a series of functions which can be utilized by other developers. Uncertainty quantification is an essential element of any quality measurement, and is utilized by these programs to both improve known measurements and to get a grasp on how well we understand a "black box" problem.

Publications

Conference Papers

Moussa, J. R., J. D. Hutchinson and G. E. I. McKenzie. Impact of Spontaneous Fission Neutron Emission Energy on Neutron Detector Response. Presented at *2021 ANS Winter Meeting and Technology Expo*. (Washington, District Of Columbia, United States, 2021-11-30 - 2021-12-04). (LA-UR-21-26462)

Reports

Cutler, T. E., A. C. Madden and G. E. I. McKenzie. Review of Neutron Uncertainty Types. Unpublished report. (LA-UR-21-28890)

Presentation Slides

Moussa, J. R., J. D. Hutchinson and G. E. I. McKenzie. Impact of Spontaneous Fission Neutron Emission Energy on Neutron Detector Response. Presented at *2021 ANS Winter Meeting and Technology Expo*, Washington, District Of Columbia, United States, 2021-11-30 - 2021-12-04. (LA-UR-21-31642)

Measuring and Modeling Void Collapse for Materials Science and Dense Plasma Regimes at the Linac Coherent Light Source

David Montgomery
20210717ER

Project Description

Understanding how mesoscale imperfections, such as voids, cracks and other defects affect material behavior under extremes such as shock loading is important to Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions for advanced material design, inertial confinement fusion, and how we model materials with computers. In this project we will obtain high resolution x-ray movies of the collapse of small voids driven by a strong shock using the x-ray laser at the Stanford Linear Accelerator Center (SLAC) National Accelerator Laboratory. Such information will help inform and improve our computational models of void collapse and how that affects material behavior important for DOE and NNSA missions, including the nuclear weapons stockpile.

Technical Outcomes

We met our project goals, and provided the Linac Coherent Light Source (LCLS) team with an idealized void collapse experiment that ended up providing some of the best measurements. Our team also strongly suggested increasing the x-ray probe energy from 8.2 keV to 18 keV, which resolved a problem with previous LCLS experiments, and allowed successful achievement of the project goals.

Publications

Journal Articles

Hodge, D., S. Pandolfi, Y. Liu, K. Li, A. Sakdinawat, M. Seaberg, P. Hart, E. Galtier, D. Khagani, S. Vetter, C. B. Curry, F. Decker, B. Nagler, H. J. Lee, C. A. Bolme, K. J. Ramos, P. M. Kozlowski, D. S. Montgomery, M. Dayton, L. Dresselhaus-Marais, S. Ali, L. D. Claus, M. O. Sanchez, T. Carver, R. L. Sandberg and A. Gleason. Visualization of Shocked Material Instabilities Using a Fast-Framing Camera and XFEL Four-Pulse Train. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-21-28603)

Presentation Slides

Montgomery, D. Quantitative X-ray Phase Contrast Imaging for Dynamic Experiments at Coherent X-ray Light Sources (Day 1) - X-ray Phase Contrast Imaging Overview, Theory, and Applications. Presented at *Institute for Materials Science Sponsored Lecture (Virtual only)*, Los Alamos, New Mexico, United States, 2021-07-20 - 2021-07-20. (LA-UR-21-26811)

Pandolfi, S., A. Gleason, H. Lee, B. Nagler, E. Galtier, E. Cunningham, Y. Liu, S. Marchesini, K. Li, A. Sakdinawat, P. Hart, C. Curry, M. H. Seaberg, D. Khaghani, S. L. Vetter, F. J. Decker, W. Mao, T. Carver, R. Sandberg, D. S. Hodge, M. Ricks, C. McCombs, N. Blanchard, D. Montgomery, C. A. Bolme, P. M. Kozlowski, K. J. Ramos, M. S. Powell, A. F. Leong, S. Ali, P. Celliers, M. Dayton, L. Dresselhaus-Marais, T. Doeppner, L. D. Claus and M. O. Sanchez. Ultrafast time-resolved imaging of void collapse in ICF ablator materials. Presented at *APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-31420)

Posters

Montgomery, D., A. F. Leong, J. L. Barber, C. A. Bolme and K. J. Ramos. In situ phase contrast imaging for cracks and voids under dynamic loading. Presented at *2021 Conventional High Explosives Grand Challenge (CHEGC) Technical Symposium*, Los Alamos, New Mexico, United States, 2021-12-06 - 2021-12-10. (LA-UR-21-31792)

Actinide Composition of Molten Salt Reactor Fuel from Fission Gases

Anna Hayes-Sterbenz
20210726ER

Project Description

For both energy security and nuclear non-proliferation it is important to be able to determine the fissile content of any nuclear reactor fuel. However, for molten salt reactors, which are increasingly being considered by the international community as a promising technology for clean and reliable energy, obtaining knowledge of the fuel content is particularly difficult. This is because many designs involve dissolving the fission fuel into the molten salt. This project aims to derive a method for deducing the content of the fission fuel from fission gases that are easily collected.

Technical Outcomes

The research in this project successfully analyzed the variation in fission product gases emitted from a molten salt reactor with uranium versus thorium fuel. In particular, variations in isotopic ratios within the fission gases Ruthenium, Krypton, and Xenon exist that can be measured through destructive analysis or by gamma ray emission non-destructively if enough efficiency exists that uncertainties are low. The work will aid nonproliferation of molten salt reactors and advanced reactor technology development.

Publications

Reports

Trellue, H. R., P. L. Lafreniere, A. Maldonado, A. C. Hayes-Sterbenz and V. K. Mehta. Determination of Actinide Composition in Molten Salt Reactors Using Fission Gases. Unpublished report. (LA-UR-21-28258)

Presentation Slides

Hayes-Sterbenz, A. C. Spectra of Antineutrinos from Nuclear Reactors. Presented at *2021 Nuclear Data for Reactor Antineutrino Measurements Workshop*, Webex, New York, United States, 2021-06-21 - 2021-06-24. (LA-UR-21-25863)

A Neural Network Framework for Kernel Density Estimator Reconstruction

Mathew Cleveland
20210728ER

Project Description

Multiphysics simulations with Monte Carlo are vital to many areas of mission space within the Department of Energy (DOE) and National Nuclear Security Administration (NNSA). This work seeks to improve the robustness and accuracy of these simulations by developing variance reduction techniques using machine learning and advanced statistical reconstructions. The goal is to provide a proof of principle for implementing neural network based kernel density estimators that can be used to increase the robustness and accuracy of multiphysics Monte Carlo simulations. Success could drastically improve these solvers as used in the DOE and NNSA complex.

Technical Outcomes

The team has shown how the novel approach of using neural networks to dynamically detect discontinuities and set bandwidths for Kernel Density Estimators. This approach can drastically reduce variance in Monte Carlo multiphysics simulations. A simple neural networks design and training procedure was developed along with a strategy for post Monte Carlo cycle smoothing reconstruction using these pre-trained networks. A simplified inertial confinement fusion (ICF) capsule simulation used used to show these improvements.

A Neutron Target at the Los Alamos Neutron Science Center

Michael Furlanetto
20210745ER

Project Description

There is presently no method to directly measure neutron-induced reactions on short-lived isotopes. These same isotope play a key role in the understanding of environments as diverse as stellar interiors, cosmic explosions, nuclear reactor fuels, and man-made nuclear explosions. In a revolutionary leap, a concept for performing these measurements by creating a dense neutron "target" using neutron spallation, like what is done at the Los Alamos Neutron Science Center (LANSCE), has been proposed. This research will perform the necessary simulation studies to understand if and how such a capability might be built at LANSCE and what its performance would be. If the results are promising, this would open the path to a completely new experimental capability at LANSCE to address outstanding questions for both basic and applied nuclear science mission.

Technical Outcomes

This project furthered a neutron target facility at the Los Alamos Neutron Science Center (LANSCE) by looking in detail at the neutron production and interaction with realistic materials for the neutron target, advancing from a thought experiment to an initial physics design. Most importantly, the characteristics of the thought experiment that offered a revolutionary advance were born out in the physics design studies. In fact, the neutron target, was shown to be feasible. This project suggested first experiments for implementation.

Publications

Reports

Mosby, S. M., A. L. Cooper, A. J. Couture, R. Reifarth and I. Dillmann. Status and prospects for the development of a Neutron Target Facility. Unpublished report. (LA-UR-21-30261)

Presentation Slides

Reifarth, R. Neutron-induced reactions in inverse kinematics. Presented at *North American Storage Rings and Neutron Captures Workshop*, virtual, Canada, 2021-06-28 - 2021-06-30. (LA-UR-21-26122)

Prediction Improvements of Transient Behavior in Advanced Reactors (PITBAR)

Holly Trellue
20210801ER

Project Description

Currently the most popular reactors operating worldwide are Light Water Reactors (LWRs), which use water as a coolant, and many codes exist to estimate performance of LWRs. Advanced reactors aim to produce power more efficiently than LWRs with more innovative coolant and fuel, but they utilize different materials and operating conditions, so not as many codes exist to predict behaviors. One area that is particularly important for safety of the system and assessing various accident scenarios in a reactor is transient calculations, or changes in neutron reactivity over minute- and hour-long time scales at startup or after changes to the system. The accuracy of tools to predict such behavior needs to be validated by neutron criticality experiments so that the codes can predict values accurately and assure that advanced reactors are safe to operate. Los Alamos National Laboratory (LANL) has strength in performing many facets of multi-physics predictive simulations for reactor designs, including neutron transport, thermal/mechanical, and fluid dynamics, but our ability in transient modeling for advanced reactors needs to be improved to be competitive in the nuclear energy community. This project will develop and validate a tool and propose future experiments that will benefit both LANL and industry.

Technical Outcomes

This project successfully developed and demonstrated multi-physics capabilities for small reactors to help Los Alamos and other individuals/companies across the nation simulate and validate performance. In particular, the team successfully modeled the dynamic aspects of the Hypatia experiment with yttrium hydride moderating material at the National Critical Experiments Research Center and matched measured performance. Additionally, the team developed methodology to link output from the world-renowned Monte Carlo N-particle transport code (MCNP) to DOE-NE/NRC-supported tools.

Publications

Reports

Blood, M. E. LANL's Microreactor Critical Testing and Demonstration Program. Unpublished report. (LA-UR-21-28344)

Blood, M. E. Hypatia Thermal Simulation Master Report. Unpublished report. (LA-UR-21-29320)

Maldonado, A., H. R. Trellue, M. E. Blood, M. E. Rising and J. G. Richard. MCNP\xc2\xae-Generated Multigroup Macroscopic Cross Section Capability for Griffin and Validation with Hypatia Experiment. Unpublished report. (LA-UR-21-29177)

Trellue, H. R., R. H. Kimpland, M. E. Blood, J. G. Richard and A. Maldonado. Prediction Improvements of Transient Behavior in Advanced Reactors (PITBAR). Unpublished report. (LA-UR-21-29180)

Presentation Slides

Grammens, J. R. LANL Microreactor High-Fidelity Modeling Advancements. . (LA-UR-21-28752)

Maldonado, A. Custom Benchmarks in Whisper, Correlation Coefficients for Microreactor Systems, MCNP \xe2\x80\x80Sensitivity Tallies to Gauge Similarity. Presented at *2021 MCNP User Symposium*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26368)

Richard, J. G. Three Fundamental Aspects of Nuclear Reactor Design. . (LA-UR-21-26206)

Rising, M. E., T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, R. A. I. Forster, C. J. Josey, J. A. Kulesza, A. J. Zukaitis, J. E. Sweezy, S. Swaminarayan and L. Casswell. Recent MCNP6(R) Code Developments and Improvements for Nuclear Engineering Applications. Presented at *2021 Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25703)

Extending High Altitude Water Cherenkov (HAWC) Science to the High and Low Energies

James Harding
20210947ER

Project Description

The Department of Energy (DOE), National Science Foundation (NSF), and National Aeronautics and Space Administration (NASA) are all funding fundamental research to investigate the nature of dark matter. The project will result in the constraint of axion-like particles (ALPs) – which are one candidate for the dark matter of the universe. Discovery of the dark matter would be a major discovery solving one of the longest standing problems in astrophysics, cosmology, and particle physics. The search for dark matter is one of the five Science Drivers from the 2014 Report of the Particle Physics Project Prioritization Panel (P5), a priority of the DOE Office of Science High-energy Physics and a highlighted opportunity for this year. Our work will push our knowledge of gamma-ray bursts (GRBs) to new energy and time domains. Observation of GRBs at teraelectronvolt (TeV) energies in the first seconds of their emission would give a look at the mechanisms that power these energetic events. Observation of the signatures of ALPs would provide evidence of the nature of the dark matter, in a regime that is currently unable to be explored in laboratories on Earth.

Technical Outcomes

As a result of this project, we now have pushed the gamma-ray burst searches with the High-Altitude Water Cherenkov (HAWC) Observatory out to more distant gamma-ray bursts and lower-energy gamma-ray burst emission. Now, even a lack of gamma-ray bursts observed with HAWC will exclude many theoretical models of gamma-ray burst emission. We have also expanded the range of axion-like particles that have been searched for on Earth, probing values of the particles that had never been able to be searched with other methods.

Resolving Transport Processes in Multispecies Plasma Shock Waves

Samuel Langendorf
20200564ECR

Project Description

This project seeks to improve the physics basis and predictive capability of Department of Energy (DOE) advanced computer codes. The project seeks to do this by obtaining detailed measurement of a plasma-shock-driven mixing process in a laboratory experiment, using novel detectors enabled by a new type of rotatable mirror array found in modern video projectors. Results are also of basic scientific interest in plasma science and astrophysics.

Publications

Presentation Slides

Keenan, B., S. Langendorf, F. Chu, A. L. LaJoie and W. Taitano. Multi-Ion Plasma Shock Formation From Colliding Supersonic Jets on the PLX. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30932)

LaJoie, A., F. Chu, L. Webster, S. Langendorf and M. Gilmore. Overview of Present and Planned Diagnostics of the Plasma Liner Experiment (PLX). Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30837)

Posters

Keenan, B., S. Langendorf, F. Chu, A. L. LaJoie and W. Taitano. Multi-Ion Plasma Shock Formation From Colliding Supersonic Jets on the PLX. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30886)

LaJoie, A., F. Chu, L. Webster, S. Langendorf and M. Gilmore. Overview of Present and Planned Diagnostics of the Plasma Liner Experiment (PLX). Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30823)

Exploring Inside the Los Alamos Neutron Science Center (LANSCE) Hydrogen- Ion Source with Laser Absorption Techniques

David Kleinjan
20200570ECR

Project Description

The high energy negative hydrogen ion beam used at the Los Alamos Neutron Science Center's (LANSCE) is created with a negative hydrogen ion source. Using optical laser techniques, we can see inside this ion source. The goal is to increase the overall beam output of LANSCE to meet critical national security needs. This project aims to develop a diagnostic tool using these optical laser techniques to improve the stability and output of the negative hydrogen ion source, and thus the performance of LANSCE. This tool not only has the potential to improve LANSCE mission needs, but once developed, could be utilized by other United States accelerator user facilities to improve their respective beam outputs.

Publications

Journal Articles

Kleinjan, D. W., G. Rouleau and L. P. Neukirch. Exploring Inside the LANSCE H- Ion Source with Laser Absorption Techniques. Submitted to *AIP Conference Proceedings*. (LA-UR-20-27331)

Presentation Slides

Kleinjan, D. W. LANL & Max Planck IPP Kickoff Discussions. . (LA-UR-20-21378)

Kleinjan, D. W. Exploring Inside the LANSCE H- Ion Source with Laser Absorption Techniques. Presented at *The 7th International Symposium on Negative Ions, Beams and Sources (NIBS'20). VIRTUAL EVENT*, Los Alamos, New Mexico, United States, 2020-09-01 - 2020-09-11. (LA-UR-20-26755)

Quantum Chromodynamics (QCD) Fragmentation Scaling Laws from Space-Time Reciprocity

Duff Neill
20200584ECR

Project Description

This work focuses on fundamental science research supported by the Department of Energy (DOE) Office of Science, developing new mathematical techniques for the systematic approximation of non-linear quantum dynamics with many degrees of freedom. This is important for advancing our basic knowledge of the universe, but beyond that, also develops capabilities to tackle and predict some of the most complicated physical processes known to humanity. Such knowledge is paramount in order to therefore prove our capabilities to engineer detectors and experiments that can produce and measure such processes (these having a diverse field of applications), while also showing how one can calculate many other related non-linear strongly interacting quantum systems.

Publications

Journal Articles

Neill, D. A. Local Parton-Hadron Duality Revisited. Submitted to *Journal of High Energy Physics*. (LA-UR-20-27861)

Kinetic Study of a Magnetic-Mirror Wet-Wood-Burner Fusion Neutron Source

Ari Le
20200587ECR

Project Description

This project studies the possibility of using a relatively simple and inexpensive magnetic mirror geometry to confine a target plasma of fusion fuel and generate fusion neutrons by bombarding the target plasma with a high-energy beam of additional fusion fuel. Such a fusion neutron source could be used to study material properties under high neutron loads, to diagnose materials, and to prepare rare isotopes for medical and other scientific research. As part of the project, we will develop high-fidelity plasma physics models in a kinetic code that can be used in future studies of fusion in magnetically-confined reactor concepts and high-energy density physics experiments conducted at pulsed power facilities.

Publications

Journal Articles

Wetherton, B. A., A. Y. Le, J. Egedal, C. Forest, W. S. Daughton, A. J. Stanier and S. Boldyrev. A drift kinetic model for the expander region of a magnetic mirror. Submitted to *Physics of Plasmas*. (LA-UR-21-20139)

Presentation Slides

Le, A. Y., B. A. Wetherton, J. Egedal, C. B. Forest, W. S. Daughton and A. J. Stanier. End Losses from a Magnetic Mirror: Kinetic Simulations and Guiding Center Theory. Presented at *APS Division of Plasma Physics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-28879)

Le, A. Y. and B. A. Wetherton. VPIC Mirror Modeling Update. . (LA-UR-21-26113)

Wetherton, B. A., A. Y. Le, A. J. Stanier, J. Egedal and C. B. Forest. Particle-in-cell Modeling of Magnetic Mirror Confinement Devices with VPIC. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30912)

Wetherton, B. A., A. Y. Le, J. Egedal, C. B. Forest, W. S. Daughton, A. J. Stanier and S. Boldyrev. A Drift Kinetic Model for the Expander Region of a Magnetic Mirror. Presented at *WHAM Physics Meeting*, Online, New Mexico, United States, 2021-03-10 - 2021-03-10. (LA-UR-21-22241)

Posters

Le, A. Y. Hybrid-VPIC 3D full-device magnetic mirror simulation preformed on Grizzly. . (LA-UR-22-20816)

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

Shocked Variable-Density Turbulence

Tiffany Desjardins
20210601ECR

Project Description

Without underground testing, we rely on simulations to validate the integrity of the nation's stockpile. Los Alamos has been developing some of the most advanced simulation codes in order to model the complex physics involved. To both improve and validate these codes, we need to develop simplified experiments that allow us to target a specific piece of physics. This project aims to study one such piece: the interaction of a shock wave with variable-density turbulence, i.e., two fluids with large density differences mixing together. This interaction occurs in supernova and inertial confinement fusion implosions. Despite years of study, we still have difficulty in accurately predicting the outcome of such systems. By studying the effects a shock has on variable-density turbulence, we can develop a physical understanding of this complex interaction. The results will be used to develop simplified models that must be integrated into our existing simulation and computing codes. Improvement of these codes will aid in the assurance of our nation's existing and future stockpile.

Diagnosing Plasma Viscosity in Compressible High-Energy-Density Systems

Joshua Sauppe
20210659ECR

Project Description

Stockpile stewardship requires a thorough understanding of how matter behaves under extreme conditions. This project will focus on improving our understanding of the plasma viscosity. In contrast to low-energy-density fluid systems, the viscosity in a weakly coupled plasma rises rapidly as the temperature increases, and viscosity is predicted to provide some stabilization of hydrodynamic instability growth which can occur in imploding systems such as inertial confinement fusion (ICF) targets. Because these instabilities can contribute to material mixing in ICF implosions, accurately capturing this growth is essential to improving the predictive capability of our radiation-hydrodynamics codes. The primary goal of this research is to develop a cylindrical implosion target design that can be used to directly measure the stabilizing effects of plasma viscosity on such instability growth. The research is expected to result in several designs that could be fielded on laser facilities in the near future, providing very useful validation data for our models in these high-energy-density regimes.

MEGAgram (Measurements of Ejecta in GAs): Digital Holography for Ejecta in Extreme Conditions

Dana Duke
20210695ECR

Project Description

As an explosively driven shock wave impacts machined grooves in a metal surface, it ejects a cloud of the material, known as "ejecta". The physics and behavior of ejecta is important for national security interests, however the experiments are challenging. Scientists must measure microscopic particles propelled by high-explosives at supersonic speeds through high temperature gas. MEGAgram (Measurements of Ejecta in GAs Holograms) will produce the first ever multi-frame digital holographic rendering of micron-scale ejecta in these national security-relevant and previously inaccessible environments. Utilizing cutting-edge laser and digital imaging technology, MEGAgram's goal is to provide scientists a multi-frame, 3-Dimensional look into evolving ejecta behavior as it moves through gas. The successful MEGAgram experiments will enable new discoveries about ejecta physics and provide new data. This mission-focused capability will help the United States Department of Energy/National Nuclear Security Administration gain a critical advantage in modeling complex, dynamic systems.

Searches for Exotic Spin-dependent Interactions using a Spin-Exchange Relaxation-Free Magnetometer and a Rare-earth Iron Garnet Mass

Pinghan Chu
20210750ECR

Project Description

This project will utilize world-leading expertise in Los Alamos in development and application of spin-exchange relaxation-free magnetometers, one of the most sensitive quantum magnetic-field sensors. While exploring exotic spin-dependent interactions between two particles, mediated by new bosonic particles, has been of keen interest in solving the most profound modern physics puzzles, such as the matter-antimatter asymmetry of the Universe and the nature of dark matter, the high energy physics (HEP) and nuclear physics communities have also developed growing interest in quantum sensing in precision measurement and discovery of new physics. Recently, Department of Energy (DOE) has announced a program in HEP-QIS, "Quantum Information Science Enabled Discovery (QuantISED)", aligned with the "Science First" driver for the national QIS program. This pioneering idea using quantum sensors with the polarized mass of zero magnetization provides a promising method for fundamental searches in nuclear physics, particle physics, and astrophysics.

Publications

Journal Articles

Chu, P., N. Ristoff, J. Smits, N. Jackson, Y. J. Kim, I. M. Savukov and V. M. Acosta. Proposal for the search for new spin interactions at the micrometer scale using diamond quantum sensors. Submitted to *Physical Review Research*. (LA-UR-22-20703)

A Multidimensional Multiscale Vlasov-Fokker-Planck Algorithm for Modeling High Energy Density and Inertial Confinement Fusion Applications

William Taitano
20190529ECR

Project Description

After the failed attempt of ignition at the National Ignition Facility (NIF), the predictive capabilities of our radiation hydrodynamic (rad-hydro) codes have been put into question. At the moment, it is not clear if the mismatch between calculations and experiments is caused by missing physics (e.g., kinetic plasma effects) in our rad-hydro codes, or inferior algorithms used therein. The project will build foundational algorithmic capabilities which will allow us to investigate the role of these 'missing physics' in our rad-hydro simulations and ultimately, increase our predictive capabilities for related laboratory experiments.

Technical Outcomes

The primary goal of extending the electrostatic ("1D2V") Vlasov adaptive phase-space grid strategy to the electromagnetic ("2D3V") setting was successful. Further, the extension demonstrated that discrete conservation of mass, momentum, and energy can be rigorously enforced in such system. With this proof-of-work serving as the basis, a fully kinetic Vlasov-based plasma simulation capability for an engineering-scale system could be developed in future work.

Publications

Reports

Taitano, W., L. Chacon and A. N. Simakov. The Annual IC Progress Report. Unpublished report. (LA-UR-20-22359)

Presentation Slides

Taitano, W. A Multiscale Eulerian Vlasov-Fokker-Planck Algorithm with Applications to High Energy Density Systems. Presented at *Virtual seminar at the Air Force Research Laboratory*, Los Alamos, New Mexico, United States, 2021-02-01 - 2021-02-01. (LA-UR-21-20616)

Taitano, W., N. Kabadi and A. Bose. iFP simulations for Omega experiments studying implosions about the cryogenic vapor pressure of 0.3 mg/cc. . (LA-UR-21-24874)

Posters

Taitano, W. A Conservative Multiscale 2D3V Curvilinear Phase-Space Moving Grid Algorithm for the Vlasov Equation with Applications to High Energy Density System. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics (Virtual Meeting)*, Los Alamos, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-29145)

Adaptive Process Control for Beyond-State-of-the-Art Alkali Antimonide Photocathodes

Vitaly Pavlenko
20190536ECR

Project Description

Hard X-ray free electron lasers such as Linac Coherent Light Source-II (LCLS-II) and Matter-Radiation Interactions in Extremes (MaRIE) are considered essential to enable sustainable stockpile stewardship. Reliable operation and performance of such billion-dollar facilities depends on a tiny but critical piece, a photocathode (laser-triggered source of electrons). Fabrication of one of the most important photocathode types, alkali antimonides, to this day remains an art, as opposed to a technological process that applies to every other part of the system. We believe that we possess the knowledge required to eliminate the vulnerability and poor reproducibility associated with a human-controlled process and deliver the first-ever fully automated photocathode growth system.

Technical Outcomes

The project demonstrated first-ever automated growth of photoemissive alkali antimonide thin films, a technique that adjusts and maintains stoichiometry of the growing film without any human interaction. The technique is robust and allows development of a new type of recipes that can be easily transferred to another photocathode thin film deposition lab/facility. The new method is potentially of interest for cold/bright photocathode R&D as well as commercial/industrial photocathode manufacturers.

Publications

Journal Articles

Alexander, A. M., M. Gaowei, S. Mistry, J. Walsh, F. Liu, K. Evans-Lutterdot, E. Stavitski, V. Pavlenko, K. Attenkofer, J. M. Smedley and N. A. Moody. Robust method for broadband efficiency enhancement of electron photocathodes using optical interferences. Submitted to *Applied Physics Letters*. (LA-UR-21-22492)

Pavlenko, V., J. M. Smedley, A. Scheinker, R. L. Fleming, A. M. Alexander, M. A. Hoffbauer and N. A. Moody.

Stoichiometry control and automated growth of alkali antimonide photocathode films by molecular beam deposition. Submitted to *Applied Physics Letters*. (LA-UR-21-30432)

Presentation Slides

Pavlenko, V. Automated growth of photocathode films: from the basics of process control towards artificial intelligence. Presented at *Photocathode Physics for Photoinjectors (P3) Workshop*, Menlo Park, California, United States, 2021-11-10 - 2021-11-12. (LA-UR-21-31176)

Pavlenko, V. Automated Growth of Photocathodes. . (LA-UR-22-20586)

Posters

Alexander, A. M., F. Liu, V. Pavlenko, N. A. Moody, J. M. Smedley and P. Bandaru. Interference Enhanced Photocathodes. Presented at *Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28528)

A Dual n-gamma Detector Array to Correct Neutron Transport Simulations

Keegan Kelly
20190588ECR

Project Description

Monte Carlo simulations of nuclear systems are essential for the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) national nuclear security missions. These simulations contain ambiguities because they include commonly-encountered neutron scattering cross sections that are poorly known, poorly measured, and estimated from nuclear models. This project aims to resolve these ambiguities by taking advantage of recent developments in detector technologies to create a detector system capable of yielding accurate and complete measurements of these cross sections and the corresponding angular distributions.

Technical Outcomes

Technical results of this project include identification of a detector type well suited for neutron-gamma ray measurements from scattering, initial design of the proposed detector array, and significant advancements in dual neutron-gamma ray data analysis techniques using liquid scintillators. The project also resulted in measurement of carbon and iron scattering with a prototype array and extraction of neutron, gamma ray, and correlated neutron-gamma ray angular distributions from the 12C(n,n') reaction measured with liquid scintillator detectors.

Publications

Journal Articles

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Correlated n-\xce\xb3 Angular Distributions from the 12C(n,n#1) Reaction for Incident Neutron Energies from 6.5–16.5 MeV. Submitted to *Physical Review C*. (LA-UR-21-21204)

Conference Papers

Kelly, K. J., M. J. Devlin and J. M. O'Donnell. Development of a Highly-Segmented Dual n-gamma Detector Array for Neutron Scattering Measurements at LANL. Presented at *SORMAWest 2020*. (Berkeley, California, United States, 2020-06-01 - 2020-06-04). (LA-UR-20-21042)

Presentation Slides

Kelly, K. J. Development in Neutron Scattering at WNR using Dual n-gamma Detection. . (LA-UR-21-23850)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. LANSCE Experimental Updates II: Neutron Scattering at WNR. Presented at *2020 Cross Section Evaluation Working Group*, Upton, New York, United States, 2020-11-30 - 2020-12-04. (LA-UR-20-29952)

Kelly, K. J., M. J. Devlin, J. M. O'Donnell and E. A. Bennett. Development of Dual n-gamma Techniques at the Los Alamos Neutron Science Center. Presented at *SORMAWest 2021*, N/A, New Mexico, United States, 2021-05-14 - 2021-05-21. (LA-UR-21-24477)

Conservative Slow-Manifold Integrators

Joshua Burby
20180756PRD4

Project Description

Physical systems and their computational modeling in national security applications often encounter extreme scale separation. The inherent stiffness in the physical models presents a grand challenge in multiscale simulations and predictive science. The current project seeks to develop a new paradigm in multiscale simulations via the so-called conservative slow manifold integrators. The key innovation is based on two fundamental properties of stiff systems that have been largely overlooked by previous investigators: (1) in the presence of irrelevant timescales, dynamics occur on invariant sets known as slow manifolds; (2) systems with conservation laws aways possess multi-linear skew-symmetric brackets that generalize Poisson brackets. Through the identification of slow manifolds, we can systematically identify dependent variables for various systems that nonlinearly separate the relevant and irrelevant timescales. In terms of those variables, we will then discretize the relevant skew-symmetric bracket in order to derive nonlinearly-implicit time integrators that preserve any number of first integrals exactly. This new advance will lead to groundbreaking simulations for topical problems in magnetic and inertial confinement fusion physics where the numerical and physical implications of stiffness are poorly understood.

Publications

Journal Articles

*Burby, J. W. Guiding center dynamics as motion on a formal slow manifold in loop space. 2020. *Journal of Mathematical Physics*. **61** (1): 12703. (LA-UR-19-24299 DOI: 10.1063/1.5119801)

Burby, J. W. Slow manifold reduction as a systematic tool for revealing the geometry of phase space. Submitted to *Physics of Plasmas*. (LA-UR-22-20125)

Burby, J. W., E. Hirvijoki and M. Leok. Nearly-periodic maps and geometric integration of noncanonical Hamiltonian systems. Submitted to *Journal of Nonlinear Science*. (LA-UR-21-32231)

Burby, J. W., J. Finn and C. L. Ellison. Improved accuracy in degenerate variational integrators for guiding center and magnetic field line flow. Submitted to *Journal of Plasma Physics*. (LA-UR-21-22168)

Burby, J. W., N. Duignan and J. Meiss. Integrability, normal forms and magnetic axis coordinates. Submitted to *Journal of Mathematical Physics*. (LA-UR-21-22030)

*Burby, J. W., N. Kallinikos and R. MacKay. Generalized Grad–Shafranov equation for non-axisymmetric MHD equilibria. 2020. *Physics of Plasmas*. **27** (10): 102504. (LA-UR-20-24232 DOI: 10.1063/5.0015420)

Burby, J. W., N. Kallinikos and R. S. MacKay. Some mathematics for quasi-symmetry. Submitted to *Journal of Mathematical Physics*. (LA-UR-19-32407)

*Burby, J. W., Q. Tang and R. Maulik. Fast neural Poincar\xc3\xa9 maps for toroidal magnetic fields. 2021. *Plasma Physics and Controlled Fusion*. **63** (2): 24001. (LA-UR-20-25019 DOI: 10.1088/1361-6587/abcbaa)

Burby, J. W., R. L. Dewar, Z. S. Qu, N. Sato and M. J. Hole. Time-dependent relaxed magnetohydrodynamics -- inclusion of cross helicity constraint using phase-space action. Submitted to *Physics of Plasmas*. (LA-UR-20-23641)

Burby, J. W., R. MacKay and N. Kallinikos. Approximate symmetries of guiding-centre motion. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-20-28555)

*Burby, J. W. and D. E. Ruiz. Variational nonlinear WKB in the Eulerian frame. 2020. *Journal of Mathematical Physics*. **61** (5): 53101. (LA-UR-19-21078 DOI: 10.1063/1.5099383)

*Burby, J. W. and E. Hirvijoki. Normal stability of slow manifolds in nearly periodic Hamiltonian systems. 2021. *Journal of Mathematical Physics*. **62** (9): 093506. (LA-UR-21-23132 DOI: 10.1063/5.0054323)

Burby, J. W. and G. Miloshevich. Hamiltonian reduction of Vlasov-Maxwell to a dark slow manifold. Submitted to *Journal of Plasma Physics*. (LA-UR-21-20381)

Burby, J. W. and J. Squire. General formulas for adiabatic invariants in nearly-periodic Hamiltonian systems. Submitted to *Journal of Plasma Physics*. (LA-UR-20-23640)

*Burby, J. W. and T. J. Klotz. INVITED: Slow manifold reduction for plasma science. 2020. *Communications in Nonlinear

Science and Numerical Simulation. **89**: 105289. (LA-UR-19-32243 DOI: 10.1016/j.cnsns.2020.105289)

*Hirvijoki, E., J. W. Burby, D. Pfefferle and A. J. Brizard. Energy and momentum conservation in the Euler–Poincar\xc3\xa9 formulation of local Vlasov–Maxwell-type systems. 2020. *Journal of Physics A: Mathematical and Theoretical*. **53** (23): 235204. (LA-UR-19-32412 DOI: 10.1088/1751-8121/ab8b38)

*Parker, J. B., J. W. Burby, J. B. Marston and S. M. Tobias. Nontrivial topology in the continuous spectrum of a magnetized plasma. 2020. *Physical Review Research*. **2** (3): 033425. (LA-UR-20-28556 DOI: 10.1103/PhysRevResearch.2.033425)

Zonta, F., R. Iorio, J. W. Burby, C. Liu and E. Hirvijoki. Dispersion relation for gauge-free electromagnetic drift kinetics. Submitted to *Physics of Plasmas*. (LA-UR-21-25075)

Reports

Klotz, T. and J. W. Burby. Slow Manifolds of fast-slow systems, the Vlasov-Maxwell System, and Control of Confined Plasma. Unpublished report. (LA-UR-19-27827)

Presentation Slides

Burby, J. W. Integrating guiding center motion in loop space. . (LA-UR-19-22767)

Burby, J. W. Compatibility Conditions for Quasisymmetry. . (LA-UR-19-27161)

Burby, J. W. Slow manifold integrators and the errors the commit. . (LA-UR-19-28965)

Burby, J. W. Slow manifold integrators: basic theory. Presented at *Nambe Meeting*, Los Alamos, New Mexico, United States, 2020-01-22 - 2020-01-22. (LA-UR-20-20600)

Burby, J. W. Slow manifold integrators: by way of computational Hamiltonian mechanics. Presented at *Structure-Preserving Geometric Discretization of Physical Systems*, Princeton, New Jersey, United States, 2020-02-17 - 2020-02-18. (LA-UR-20-21533)

Burby, J. W. Principles for implicit integration. . (LA-UR-21-25414)

Burby, J. W. Slow manifold reduction as a systematic tool for revealing the geometry of phase space. Presented at *APS DPP*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-30788)

Burby, J. W., E. Hirvijoki and M. Leok. Geometric integration of Hamiltonian systems on exact symplectic manifolds. . (LA-UR-21-31371)

Burby, J. W., N. Kallinikos and R. MacKay. Grad-Shafranov equation for non-axisymmetric MHD equilibria. . (LA-UR-20-24872)

Burby, J. W., Q. Tang and R. Maulik. Computing Poincare maps using physics-informed deep learning. . (LA-UR-20-25536)

Burby, J. W., Q. Tang and R. Maulik. Fast neural Poincare maps for toroidal magnetic fields. Presented at *SIAM Conference on Computational Science and Engineering*, Fort Worth, Texas, United States, 2021-03-01 - 2021-03-01. (LA-UR-21-21970)

Burby, J. W. and Q. Tang. Fast neural Poincare maps for toroidal magnetic fields. . (LA-UR-20-24873)

Posters

Burby, J. W. Slow manifold integrator for electromagnetic PIC. Presented at *2019 APS DPP meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30654)

State-of-the-Art Predictions for the Matter-Antimatter Asymmetry

Christopher Lee
20190622PRD2

Project Description

This project addresses two of the great open scientific questions of our day, which are also two of the top research priorities of the Department of Energy Office of Science: "What is the origin of the matter-antimatter asymmetry?" and "What lies beyond the Standard Model of Particle Physics?" The first question addresses the origin of all visible matter in our universe today, which cannot be explained by the current Standard Model of Particle physics, thus connecting it to the second question. Answers to these require the development of frontier theoretical and computational tools as well as experimental techniques to probe physical phenomena lying beyond the Standard Model that could provide these answers. In addition, the theoretical tools are applicable to studying other physical systems, such as supernovae and how the propagation of neutrinos through them affects the dynamics of their explosions, while the experiments develop cutting-edge technology and capabilities in accelerator science and in trapping and measuring precisely ultracold neutrons. At the conclusion of our project, besides having such new tools and capabilities, we expect to have made a major step towards understanding how the matter in the universe could have been generated in its first few moments of existence.

Publications

Journal Articles

*Cheng-Wei, C., G. Cottin, D. Yong, K. Fuyuto and M. J. Ramsey-Musolf. Collider probes of real triplet scalar dark matter. 2021. *Journal of High Energy Physics*. **2021** (1): 198. (LA-UR-20-22358 DOI: 10.1007/JHEP01(2021)198)

*F. K. *. L. C. *. M. E. *. Y. B. Cirigliano, V. *., V. Cirigliano, K. Fuyuto, C. Lee, E. Mereghetti and B. Yan. Charged lepton flavor violation at the EIC. 2021. *Journal of High Energy Physics*. **2021** (3): 256. (LA-UR-21-20531 DOI: 10.1007/JHEP03(2021)256)

*Fuyuto, K., J. De Vries, P. Draper, J. Kozaczuk and B. Lillard. Uncovering an axion mechanism with the EDM portfolio. 2021. *Physical Review D*. **104** (5): 055039. (LA-UR-21-26248 DOI: 10.1103/PhysRevD.104.055039)

Fuyuto, K., V. Cirigliano, M. Ramsey-Musolf and E. Rule. Next-to-leading order scalar contributions to mu to e conversion. Submitted to *Physical Review C*. (LA-UR-21-32420)

*Fuyuto, K., W. Hou and E. Senaha. Cancellation mechanism for the electron electric dipole moment connected with the baryon asymmetry of the Universe. 2020. *Physical Review D*. **101** (1): 011901. (LA-UR-19-30968 DOI: 10.1103/PhysRevD.101.011901)

Mereghetti, E., K. Fuyuto, V. Cirigliano, W. Dekens, J. de Vries and R. Ruiz. The muon's anomalous magnetic moment in nuSMEFT. Submitted to *Physical Review D*. (LA-UR-21-24456)

*Mereghetti, E., K. Fuyuto, W. G. Dekens, J. de Vries and G. Zhou. Sterile neutrinos and neutrinoless double beta decay in effective field theory. 2020. *Journal of High Energy Physics*. **2020** (6): 97. (LA-UR-20-21376 DOI: 10.1007/JHEP06(2020)097)

Presentation Slides

Fuyuto, K. Theory Overview of Electric Dipole Moment. Presented at *Third Nuclear and Particle Theory Meeting*, St Louis, Michigan, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-24421)

Fuyuto, K. Search for lepton flavor violation at the EIC. Presented at *PPC 2021: XIV International Workshop on Interconnections between Particle Physics and Cosmology*, Norman, Oklahoma, United States, 2021-05-17 - 2021-05-17. (LA-UR-21-24724)

Fuyuto, K. Electroweak Baryogenesis in General Two Higgs Doublet Model. Presented at *Computations that Matter 2021*, Leiden, Netherlands, 2021-06-21 - 2021-06-21. (LA-UR-21-25750)

Fuyuto, K. Neutrinoless double beta decay with light sterile neutrinos. Presented at *A Virtual Tribute to Quark Confinement and the Hadron Spectrum 2021*, Virtual, Norway, 2021-08-02 - 2021-08-06. (LA-UR-21-27455)

Fuyuto, K. Fundamental symmetry tests in the lepton sector. . (LA-UR-21-31645)

Fuyuto, K. The Mystery of the Matter in the Universe. . (LA-UR-21-31644)

Fuyuto, K. Searches for violations of fundamental symmetries. . (LA-UR-22-20417)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-20967)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22082)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22446)

Fuyuto, K. Searching for new physics in violations of fundamental symmetries. . (LA-UR-22-22469)

Fuyuto, K. A cross-frontier quest to reveal the origin of the Universe. . (LA-UR-22-22561)

Searching for Dark Matter with Fixed Target Experiments

Daniele Spier Moreira Alves
20190626PRD2

Project Description

The high level goal is explore the theory and interpretation of experimental data to discover the nature of dark matter in the Universe, an unknown form of matter in galaxies that is six times more abundant than ordinary matter. The expected outcome is a further understanding of the fundamental constituents of the Universe, either by discovering new forms of matter, of by ruling out existing theories that attempt to explain dark matter. This project addresses the challenges defined as high priority scientific goals by the Department of Energy Office of Science (DOE SC) Particle Physics Project Prioritization Panel (a subpanel of the High Energy Physics Advisory Panel), the 2015 Department of Energy Office of Science (SC) Nuclear Physics Long-Range Plan, and the Laboratory's Strategic Investment Plan, specifically in its Nuclear and Particle Futures pillar.

Publications

Journal Articles

*Berlin, A., P. deNiverville, A. Ritz, P. Schuster and N. Toro. Sub-GeV dark matter production at fixed-target experiments. 2020. *Physical Review D*. **102** (9): 095011. (LA-UR-20-22261 DOI: 10.1103/PhysRevD.102.095011)

deNiverville, P., H. Lee and Y. Lee. New searches at the reactor experiments based on the dark axion portal. Submitted to *Physical Review D*. (LA-UR-21-20328)

deNiverville, P., L. Buonocore and C. Frugiuele. The hunt for sub-GeV dark matter at neutrino facilities: a survey of past and present experiments. Submitted to *Journal of High Energy Physics*. (LA-UR-19-32644)

Presentation Slides

deNiverville, P. Searching for Light Dark Matter with Fixed Target Neutrino Experiments. Presented at *T-2 Group Meeting*, Los Alamos, New Mexico, United States, 2021-01-21 - 2021-01-21. (LA-UR-21-20483)

deNiverville, P. MCNP Physics Model Comparison. Presented at *CCM Analysis Meeting*, Los Alamos, New Mexico, United States, 2021-02-11 - 2021-02-11. (LA-UR-21-21358)

deNiverville, P. DM searches in neutrino beam experiments - near and far detectors. Presented at *Workshop on Interplay of Neutrino and Dark matter Experiments and Exotic Searches*, Suwon, Korea, South, 2021-03-18 - 2021-03-19. (LA-UR-21-22524)

deNiverville, P. Changes to Coherent Dark Matter Nucleus Scattering. Presented at *CCM Analysis Meeting*, Los Alamos, New Mexico, United States, 2021-04-29 - 2021-04-29. (LA-UR-21-24075)

deNiverville, P. Searching for Dark Matter with Neutrino Experiments. Presented at *T-Division Presentations*, Los Alamos, New Mexico, United States, 2021-06-16 - 2021-06-16. (LA-UR-21-25550)

A Study of Diffusion Around Pulsar Wind Nebulae

Kelly Malone
20200684PRD2

Project Description

Department of Energy (DOE), National Science Foundation (NSF), and National Aeronautics Space Administration (NASA) are all funding fundamental research to investigate the nature of dark matter. This project will result in the constraint of pulsar wind nebulae - one of the largest backgrounds in cosmic-ray dark matter searches. With these constraints, some dark matter models can be ruled out if no residual dark matter signal is detected. If positive signal is detected, then this enables experiments such as the High Altitude Water Cherenkov (HAWC) observatory to verify that such a signal is consistent with expected dark matter behavior. Discovery of dark matter would solve one of the longest standing problems in astrophysics, cosmology, and particle physics. These studies could also explain the unusually high density of cosmic electrons around the Earth and, potentially, will indicate the sources of the highest-energy cosmic particles in the Galaxy. The techniques used reduce trillions of events to only a few hundred high-energy gamma-rays and have broad applicability in other analyses around the Laboratory. This, along with searching for small signal in a noisy dataset and dealing with large datasets (over 4 petabytes of data) all are also extendable to the Lab's stockpile stewardship mission.

Publications

Journal Articles

Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-25495 DOI: 10.22323/1.395.0810)

Malone, K. A. A search for spectral hardening in HAWC sources above 56 TeV. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-25494 DOI: 10.22323/1.395.0811)

Malone, K. A., D. A. Burgess, K. Mori, J. D. Gelfand, C. J. Hailey, Y. M. Tokayer, J. Woo, H. An, S. P. Reynolds, S. Safi-Harb and T. Temim. The Eel Pulsar Wind Nebula: a Pevatron-Candidate Origin for HAWC J1826-128 and HESS J1826-130. Submitted to *Astrophysical Journal*. (LA-UR-21-30784)

Malone, K. A., J. P. Harding, A. Albert, M. Durocher, S. Casanova, D. Huang, F. Salesa Greus, B. L. Dingus, G. J. Kunde, C. Brisbois and H. Zhou. Evidence of 200 TeV photons from HAWC J1825-134. Submitted to *Nature Astronomy*. (LA-UR-20-28703)

Malone, K. A., J. P. Harding, B. L. Dingus, M. Durocher, A. Albert, H. Zhou, C. Brisbois and V. Baghmanyan. Evidence that Ultra-High-Energy Gamma Rays are a Universal Feature Near Powerful Puslars. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-20344)

Malone, K. A. and B. L. Dingus. Multi-wavelength observations of 2HWC J1928+177: dark accelerator or new TeV gamma-ray binary?. Submitted to *Astrophysical Journal*. (LA-UR-20-28702)

Mori, K., H. An, K. A. Malone, C. Hailey, B. Humensky, B. L. Dingus, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR broad-band X-ray observational campaign of energetic pulsar wind nebulae in synergy with VERITAS, HAWC and Fermi gamma-ray telescopes. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-26689 DOI: 10.22323/1.395.0963)

Mori, K., H. An, K. A. Malone, C. Hailey, B. Humensky, B. L. Dingus, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR broad-band X-ray observational campaign of energetic pulsar wind nebulae in synergy with VERITAS, HAWC and Fermi gamma-ray telescopes. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-26689 DOI: 10.22323/1.395.0963)

Presentation Slides

Malone, K. A. Highest-energy gamma-ray emission from HAWC in the environments of powerful pulsars. Presented at *APS April Meeting*, Virtual, New Mexico, United States, 2020-04-18 - 2020-04-21. (LA-UR-20-22825)

Malone, K. A. HAWC results on other TeV halos. Presented at *1st Workshop on Gamma-ray Halos around Pulsars*, Rome (Virtual), Italy, 2020-12-01 - 2020-12-03. (LA-UR-20-29726)

Malone, K. A. Observation of the highest-energy gamma rays with the HAWC Observatory. Presented at *P-3 seminar*, Virtual, New Mexico, United States, 2021-03-25 - 2021-03-25. (LA-UR-21-22661)

Malone, K. A. Observation of the highest-energy gamma rays with the HAWC Observatory. . (LA-UR-21-23951)

Malone, K. A. Recent results from the HAWC Observatory. Presented at *Seminar to be given to the Astroparticles and Cosmology Laboratory at the University of Paris next week*, Virtual, New Mexico, United States, 2021-05-05 - 2021-05-05. (LA-UR-21-24196)

Malone, K. A. Flash poster talk for "A search for spectral hardening in HAWC sources above 56 TeV". Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25496)

Malone, K. A. The Ultra-High-Energy Source MGRO J1908+06. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25532)

Malone, K. A. HAWC study of the ultra-high-energy gamma-ray source MGRO J1908+06. Presented at *APS April 2021*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-17. (LA-UR-21-23172)

Malone, K. A. HAWC's view of the highest-energy gamma-ray sky. Presented at *19th Divisional Meeting of the High Energy Astrophysics Division of the American Astronomical Society*, Pittsburgh, Pennsylvania, United States, 2022-03-13 - 2022-03-17. (LA-UR-22-21960)

Malone, K. A., K. Mori, B. L. Dingus, H. An, C. J. Hailey, B. Humensky, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR X-ray observation campaign of energetic pulsar wind nebulae. Presented at *International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-26302)

Malone, K. A., K. Mori, B. L. Dingus, H. An, C. J. Hailey, B. Humensky, R. Mukherjee, S. Reynolds and S. Safi-Harb. NuSTAR X-ray observation campaign of energetic pulsar wind nebulae. Presented at *International Cosmic Ray Conference*, Berlin, Germany, 2021-07-12 - 2021-07-23. (LA-UR-21-26302)

Posters

Malone, K. A. A search for spectral hardening in HAWC sources above 56 TeV. Presented at *International Cosmic Ray Conference*, Virtual, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-25493)

Towards Data Science Driven Multi-physics Modeling to Probe Neutron Star Mergers

Jonah Miller
20200687PRD2

Project Description

Modeling the aftermath of neutron star mergers is of critical importance to the scientific community and helps answer fundamental questions such as the nature of matter at high density and the origin of heavy elements in the universe. The previous work at Los Alamos National Lab has not only placed it at the forefront of this effort, but it has also highlighted the many uncertainties that remain uncontrolled in current models. This work will help maintain Los Alamos National Lab's place as a world leader in this field. This project aims to solve a problem that requires a deep understanding of the complex interplay of many processes and an analysis of a high-dimensional dataset. This class of problem is broadly relevant to key laboratory mission areas.

Publications

Journal Articles

De, S. and D. M. Siegel. Igniting weak interactions in neutron-star post-merger accretion disks. Submitted to *Astrophysical Journal*. (LA-UR-20-28607)

Presentation Slides

De, S. Probing neutron stars with gravitational wave observations. Presented at *Los Alamos Astro Seminar*, Los Alamos, New Mexico, United States, 2021-03-04 - 2021-03-04. (LA-UR-21-22413)

De, S. Project visit LDRD 20200687PRD2. . (LA-UR-21-24500)

De, S. Tidal deformabilities and radii of neutron stars from gravitational-wave observations. Presented at *ECT workshop*, Virtual, Italy, 2021-06-14 - 2021-06-14. (LA-UR-21-25488)

De, S. Probing neutron star mergers with gravity and light. Presented at *Free Mesons Seminar, TIFR Bombay*, Virtual, India, 2021-07-22 - 2021-07-22. (LA-UR-21-27041)

De, S. Parameter estimation for experiments in astrophysics and hydrodynamics: techniques and infrastructures. Presented at *ANSI Seminar*, Los Alamos, New Mexico, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-30094)

De, S. and D. M. Siegel. Igniting weak interactions in neutron star post merger accretion disks. Presented at *American Physical Society April Meeting 2021*, Virtual, New Mexico, United States, 2021-04-17 - 2021-04-20. (LA-UR-21-23687)

Smullen, R. A. and S. De. Black Holes, Crashing Galaxies, and Strange New Planets. . (LA-UR-21-25276)

Decipher the Coupled Plasma and Atomic Physics for Reactor Plasma Exhaust

Xianzhu Tang
20200753PRD3

Project Description

This project addresses a key scientific and technological challenge in tokamak fusion energy, which if successful, provides a viable emission-free energy source that is a long-term solution to both energy security and climate change. The high-level goals are to understand how detailed atomic physics can impact the plasma exhaust and sustained operation of the steady-state fusion reactor, with the programmatic aim of building the fundamental physics basis for design options and constraints. The approach is to incorporate the state-of-the-art atomic data through a collisional-radiative model into plasma transport modeling, using both the kinetic and fluid approaches. The general scientific problem of how neutrals, plasmas, and radiation interact in a fusion plasma with higher standard deviations from the mean (z-score) impurity is of interest to the inertial confinement fusion problem that is a critical part of the Department of Energy/National Nuclear Security Administration missions. Although the densities are drastically different between the two applications, the fundamental physics approaches and modeling technique are of interests to both applications.

Publications

Presentation Slides

Zhang, Y. Director's postdoc fellow. . (LA-UR-22-21371)

The Urge to Merge: The Fate of Binary Black Holes

Hui Li
20200772PRD4

Project Description

When two black holes get close to each other, whether they will eventually merge or move apart is one of the outstanding questions in modern day astronomy. If they merge, they can produce gravitational waves (GW) signals seen currently by the Laser Interferometer Gravitational-Wave Observatory (LIGO) (for stellar mass black hole binaries), and possibly by Laser Interferometer Space Antenna (LISA (for supermassive black hole binaries)) in the future. The proposed work will produce comprehensive simulations of these sources and develop new tools for high performance computing. It will contribute to the Unites States' LIGO mission and future space-based international LISA mission.

Publications

Journal Articles

F. Calcino, J. P., D. J. Price, H. Garg, B. J. Norfolk, C. Pinte and H. Li. Observational Signatures of Circumbinary Discs I: Theory. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-30251)

F. Calcino, J. P., T. Hilder, D. J. Price, C. Pinte and B. J. Norfolk. Mapping the Planetary Wake in HD~163296 with Kinematics. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-31084)

Poblete, P., N. Cuello, S. Perez, S. Marino, J. P. F. Calcino, E. Macias, A. Ribas, A. Zurlo, J. Cuadra, M. Montesinos, S. Zuniga-Fernandez and A. Bayo. The protoplanetary disc around HD 169142: circumstellar orcircumbinary?. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-24101)

Verrios, H. J., D. J. Price, C. Pinte and J. P. F. Calcino. Kinematic evidence for an embedded planet in the IM Lupi disc. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-31387)

Searching for New Physics at the Intensity Frontier at the EIC

Christopher Lee
20200775PRD4

Project Description

This project will advance our ability to discover new elementary particles and forces with high-energy particle colliders, especially the upcoming Electron-Ion Collider (EIC), which will place the United States (US) at the forefront of worldwide high-energy electron-proton collider technology. We will perform the theoretical calculations, using the most modern tools in quantum field theory, to predict and optimize the sensitivity of the EIC to new physics interactions that may violate "charged lepton flavor conservation", leading to phenomena like electrons re-emerging in these collisions as heavier leptons like muons or tau leptons. Discovering and characterizing the origin of such new interactions would shed light on some of the most pressing and puzzling problems in fundamental physics today, such as where neutrino masses come from or how the excess of matter over antimatter in our universe originated. Our work will result in better guidance for detector design and optimization at EIC to find charged lepton flavor changing events, and optimize the strategies to analyze data to discover and characterize the underlying origin of such new phenomena. It will contribute to the worldwide impact of the US nuclear physics effort in collider physics.

Publications

Journal Articles

*F. K. *. L. C. *. M. E. *. Y. B. Cirigliano, V. *., V. Cirigliano, K. Fuyuto, C. Lee, E. Mereghetti and B. Yan. Charged lepton flavor violation at the EIC. 2021. *Journal of High Energy Physics*. **2021** (3): 256. (LA-UR-21-20531 DOI: 10.1007/JHEP03(2021)256)

Dong, H., P. Sun, B. Yan and C. P. Yuan. Probing the $Zb\bar{b}$ anomalous couplings via exclusive Z boson decay. Submitted to *PLB*. (LA-UR-22-20027)

Li, H. T., B. Yan and C. P. Yuan. Jet Charge: A new tool to probe the anomalous Zbb couplings at the HERA and EIC. Submitted to *PLB*. (LA-UR-21-31134)

Liu, y. and B. Yan. Searching for the axion-like particle at the EIC. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-21-31766)

Yan, B. Determining Higgs boson width at electron-positron colliders. 2021. *Physics Letters B*. **822**: 136709. (LA-UR-21-24315 DOI: 10.1016/j.physletb.2021.136709)

Yan, B. Probing the dark photon via polarized DIS scattering at the HERA and EIC. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-22-21939)

Y. Z. *. Y. C. Yan, B. *. and B. Yan. The anomalous Zbb couplings at the HERA and EIC. 2021. *Physics Letters B*. **822**: 136697. (LA-UR-21-26072 DOI: 10.1016/j.physletb.2021.136697)

Yan, B., Y. Liu and R. Zhang. Loop induced top quark FCNC through top quark and dark matter interactions. Submitted to *JHEP*. (LA-UR-21-22425)

*Yan, B. and C. P. Yuan. Anomalous Zbb Couplings: From LEP to LHC. 2021. *Physical Review Letters*. **127** (5): 51801. (LA-UR-21-20373 DOI: 10.1103/PhysRevLett.127.051801)

*Yan, B. and K. Xie. Probing the electroweak symmetry breaking with Higgs production at the LHC. 2021. *Physics Letters B*. **820**: 136515. (LA-UR-21-24074 DOI: 10.1016/j.physletb.2021.136515)

Presentation Slides

Lee, C., B. Yan, B. Yoon, G. Bell, Y. Makris and J. Talbert. Angularities, gaps, and \\alpha_s. Presented at *World SCET 2021*, Cambridge, Massachusetts, United States, 2021-04-19 - 2021-04-23. (LA-UR-21-23742)

Lee, C., B. Yoon, B. Yan, Y. Makris, J. Talbert and G. Bell. Event shape tails and alpha_s. Presented at *INT Workshop on Probing QCD at High Energy and Density with Jets*, Seattle, Washington, United States, 2021-08-09 - 2021-08-13. (LA-UR-21-27921)

Lee, C., E. Mereghetti and B. Yan. Searching for New Physics at the Intensity Frontier at the EIC: Project Visit. . (LA-UR-21-29821)

Yan, B. From Precision calculation to new physics searches at colliders. . (LA-UR-21-22158)

Yan, B., C. Lee, V. Cirigliano, K. Fuyuto and E. Mereghetti. Searching for Charged Lepton Flavor Violation at the EIC. Presented at *IAS Program on High Energy Physics*

2021, Hong-Kong, China, 2021-01-14 - 2021-01-21. (LA-UR-21-20485)

Next Generation Simulations of the Remarkable Deaths of Massive Stars

Joshua Dolence
20210808PRD1

Project Description

A wide variety of national security challenges require sophisticated computer simulations of phenomena that happen on a wide range of length and time scales. These multi-scale challenges are particularly difficult and developing expertise in this space will be broadly useful for national security applications in the future. To develop this expertise, this work will pursue cutting-edge astrophysics research, studying the explosive deaths of massive stars and making predictions for observations with a variety of facilities.

Publications

Journal Articles

J. Fields, C. E. The Three-dimensional Collapse of a Rapidly Rotating 16 M\xe2\x8a\x99 Star. 2022. *The Astrophysical Journal Letters*. **924** (1): L15. (LA-UR-21-31677 DOI: 10.3847/2041-8213/ac460c)

Fields, C. E. and S. M. Couch. Three-dimensional Hydrodynamic Simulations of Convective Nuclear Burning in Massive Stars Near Iron Core Collapse. 2021. *The Astrophysical Journal*. **921** (1): 28. (LA-UR-21-26198 DOI: 10.3847/1538-4357/ac24fb)

Presentation Slides

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-21-24999)

J. Fields, C. E. Assessing the Impact of Uncertainties in Stellar Models. Presented at *INT Program 21-3 - Radionuclides*, SEATTLE, Washington, United States, 2021-10-14 - 2021-10-14. (LA-UR-21-30143)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-21-32036)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-22-20894)

J. Fields, C. E. Next-Generation Simulations of The Remarkable Deaths of Massive Stars. . (LA-UR-22-21110)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-22-21390)

J. Fields, C. E. NEXT-GENERATION SIMULATIONS OF THE REMARKABLE DEATHS OF MASSIVE STARS. . (LA-UR-22-22147)

Supermassive Black Holes and Their Environment

Jarrett Johnson
20210942PRD2

Project Description

The Universe shows us a history that begins with a nearly uniform landscape of gas and dark matter that evolves into a field of non-linear and complex galaxies. A key component of galaxy formation is the seeding and growth of supermassive black holes, now confirmed to exist at the center of nearly all large galaxies. Understanding how these objects form would answer one of most pressing astrophysical questions of the last several decades: Must we invoke new physics to explain the existence of supermassive black holes at early times? This research will provide a theoretical understanding of black hole growth via the interaction between supermassive black holes (SMBHs) and their gaseous environments. It will (1) show that there are observational signatures of primordial black holes as SMBH seeds and (2) determine the impact of radiation from the first galaxies on SMBH assembly. Multiscale modeling of challenging astrophysical problems, like this one, builds capabilty for modeling of the high-energy density environment of nuclear explosions.

Publications

Journal Articles

Johnson, J. L. and P. R. Upton Sanderbeck. A Simple Condition for Sustained Super-Eddington Accretion. Submitted to *Astrophysical Journal*. (LA-UR-22-20494)

Upton Sanderbeck, P. R., S. Bird and Z. Haiman. Nucleosynthetic signatures of primordial origin around supermassive black holes. Submitted to *Physical Review D*. (LA-UR-21-30107)

Presentation Slides

Upton Sanderbeck, P. R. Signatures of primordial origins around supermassive black holes. . (LA-UR-22-20491)

Upton Sanderbeck, P. R. HeII reionization in simulations + (SMBH growth and reionization). Presented at *Reionization and Cosmic Dawn: Looking Forward to the Past*, Berkeley, California, United States, 2022-03-21 - 2022-03-23. (LA-UR-22-22457)

Mega Electron Volt (MeV) Gamma-Ray Astronomy: Exploring the Universe in the Nuclear Transition Region

Lucas Parker
20170693PRD4

Project Description

The development of more sensitive space-based instruments for the detection of gamma-ray and neutron emission generated by nuclear reactions is important for Department of Energy/National Nuclear Security Administration national security programs. This project will develop new tools for imaging sources of gamma-ray and neutron emission that will allow the detection and measurement of sources that are currently too faint to detect. The project will also explore new approaches to the reduction of detector background noise that will enable the construction of more sensitive gamma-ray and fast neutron detectors. Our development of these new tools for on-board Compton gamma-ray imaging and background reduction is likely to influence future designs of Space-based Nuclear Detonation Detection (SNDD) instrumentation.

Technical Outcomes

This project pioneered low-power gamma-ray data analysis techniques. Specifically, the team created a complete, end-to-end Compton analysis pipeline, realized completely in firmware. This pipeline performs Compton event reconstruction and produces full-sky images using Compton back-projection. This is a new technology for imaging in the megaelectron volt (MeV), where Compton scattering is the dominant interaction. As the pipeline is field-programmable gate array (FPGA)-based, it enables low size-weight-and-power (SWaP) gamma-ray instruments to produce images in near real-time.

Publications

Journal Articles

*Appel, J. W., Z. Xu, I. L. Padilla, K. Harrington, B. Pradenas Marquez, A. Ali, C. L. Bennett, M. K. Brewer, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. Couto, S. Dahal, K. Denis, R. Dunner, J. R. Eimer, T. Essinger-Hileman, P. Fluxa, D. Gothe, G. C. Hilton, J. Hubmayr, J. Iuliano, J. Karakla, T. A. Marriage, N. J. Miller, C. Nunez, L. Parker, M. Petroff, C. D. Reintsema, K. Rostem, R. W. Stevens, D. A. N. Valle, B. Wang, D. J. Watts, E. J. Wollack and L. Zeng. On-sky Performance of the CLASS Q-band Telescope. 2019. *The Astrophysical Journal*. **876** (2): 126. (LA-UR-18-30124 DOI: 10.3847/1538-4357/ab1652)

*Kusaka, A., J. Appel, T. Essinger-Hileman, J. A. Beall, L. E. Campusano, H. Cho, S. K. Choi, K. Crowley, J. W. Fowler, P. Gallardo, M. Hasselfield, G. Hilton, S. P. Ho, K. Irwin, N. Jarosik, M. D. Niemack, G. W. Nixon, M. Nolta, L. A. J. Page, G. A. Palma, L. Parker, S. Raghunathan, C. D. Reintsema, J. Sievers, S. M. Simon, S. T. Staggs, K. Visnjic and K. Yoon. Results from the Atacama B-mode Search (ABS) experiment. 2018. *Journal of Cosmology and Astroparticle Physics*. **2018** (09): 5-5. (LA-UR-18-23879 DOI: 10.1088/1475-7516/2018/09/005)

*Li, Z., S. Naess, S. Aiola, D. Alonso, J. W. Appel, J. R. Bond, E. Calabrese, S. K. Choi, K. T. Crowley, T. Essinger-Hileman, S. M. Duff, J. Dunkley, J. W. Fowler, P. Gallardo, S. -. P. Ho, J. Hubmayr, A. Kusaka, T. Louis, M. S. Madhavacheril, J. McMahon, F. Nati, M. D. Niemack, L. Page, L. Parker, B. Partridge, M. Salatino, J. L. Sievers, C. Sifon, S. M. Simon, S. T. Staggs, E. Storer and E. J. Wollack. The cross correlation of the ABS and ACT maps. 2020. *Journal of Cosmology and Astroparticle Physics*. **2020** (09): 10-10. (LA-UR-20-21154 DOI: 10.1088/1475-7516/2020/09/010)

Parker, L. P., S. Dahal, M. K. Brewer, A. Ali, J. W. Appel, C. L. Bennett, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. D. Couto, R. Datta, K. L. Denis, J. Eimer, F. Espinoza, T. Essinger-Hileman, D. Gothe, K. Harrington, J. Iuliano, T. A. Marriage, S. Novack, C. Nunez, I. L. Padilla, M. Petroff, R. Reeves, G. Rhoades, K. Rostem, D. A. N. Valle, D. J. Watts, E. J. Wollack and Z. Xu. Venus Observations at 40 and 90 GHz with CLASS. Submitted to *Planetary Science Journal*. (LA-UR-20-28472)

*Watts, D. J., B. Wang, A. Ali, J. W. Appel, C. L. Bennett, D. T. Chuss, S. Dahal, J. R. Eimer, T. Essinger-Hileman, K. Harrington, G. Hinshaw, J. Iuliano, T. A. Marriage, N. J. Miller, I. L. Padilla, L. Parker, M. Petroff, K. Rostem, E. J. Wollack and Z. Xu. A Projected Estimate of the Reionization Optical Depth Using the CLASS Experiment's Sample Variance Limited E-mode Measurement. 2018. *The*

Astrophysical Journal. **863** (2): 121. (LA-UR-18-20165 DOI: 10.3847/1538-4357/aad283)

Conference Papers

Dahal, S., A. Ali, J. W. Appel, T. Essinger-Hileman, C. Bennett, M. Brewer, R. Bustos, M. Chan, D. Chuss, J. Cleary, T. Engelhoven, P. Fluxa, F. Colazo, J. Couto, K. Denis, R. Dunner, J. Eimer, M. Halpern, K. Harrington, K. Helson, G. Hilton, G. Hinshaw, J. Hubmayr, J. Iuliano, J. Karakla, B. Marquez, T. Marriage, J. McMahon, N. Miller, C. Nunez, I. Padilla, G. Palma, L. P. Parker, M. Petroff, R. Reeves, C. Reintsema, K. Rostrem, M. Sagliocca, K. U-Yen, D. Valle, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan and L. Zeng. Design and Characterization of Cosmology Large Angular Scale Surveyor (CLASS) 93 GHz Focal Plane. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-24478)

Harrington, K., J. Eimer, D. Chuss, M. Petroff, J. Cleary, M. DeGeorge, A. Ali, J. W. Appel, C. Bennett, M. Brewer, R. Bustos, M. Chan, J. Couto, K. Denis, R. Dunner, T. Essinger-Hileman, P. Fluxa, M. Halpern, G. Hilton, G. Hinshaw, J. Hubmayr, J. Iuliano, J. Karakla, T. Marriage, J. McMahon, N. Miller, C. Nunez, I. Padilla, G. Palma, L. P. Parker, B. Marquez, R. Reeves, C. Reintsema, K. Rostem, D. Valle, T. Engelhoven, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan and L. Zeng. Variable-delay Polarization Modulators for the CLASS Telescopes. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-24622)

Iuliano, J., J. Eimer, L. P. Parker, A. Ali, J. W. Appel, C. Bennett, M. Brewer, R. Bustos, D. Chuss, J. Cleary, J. Couto, S. Dahal, K. Denis, R. Dunner, T. Essinger-Hileman, P. Fluxa, M. Halpern, K. Harrington, K. Helson, G. Hilton, G. Hinshaw, J. Hubmayr, J. Karakla, T. Marriage, N. Miller, J. McMahon, C. Nunez, I. Padilla, G. Palma, M. Petroff, B. Marquez, R. Reeves, C. Reintsema, K. Rostem, D. Valle, T. Engelhoven, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan and L. Zeng. The Cosmology Large Angular Scale Surveyor Receiver Design. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-25031)

Parker, L. P., S. Griffin, C. Kierans, A. Schoenwald, P. Shawhan, R. Caputo, J. McEnery and J. Perkins. Current Status of the ComPair Silicon Tracker. Presented at *SPIE Astronomical Telescopes + Instrumentation (digital, remote)*. (Los Alamos, New Mexico, United States, 2020-12-16 - 2020-12-16). (LA-UR-20-29832)

Presentation Slides

Parker, L. P. An FPGA-based Compton Mapping Pipeline. . (LA-UR-20-30237)

Posters

Parker, L. P., S. Grifffin, C. Kierans, A. Shoenwald, P. Shawhan, R. Caputo, J. McEnery and J. Perkins. Progress towards the Silicon Tracker for the All-sky Medium Energy Gamma-ray Observatory Prototype. Presented at *IEEE Nuclear Science Symposium (NSS) and Medical Imaging Conference (MIC)*, Manchester, United Kingdom, 2019-10-26 - 2019-11-02. (LA-UR-19-30803)

Matter and Nuclei at Neutron-Rich Extremes

Ingo Tews
20190617PRD1

Project Description

The work will involve large-scale calculations of atomic nuclei and of dense nucleonic matter present in neutron stars. Advancing our ability to calculate the properties and reactions of atomic nuclei will allow us to advance the state of the art in predicting nuclear reactions in regimes where experiments are difficult or impossible, like reactions on unstable nuclei.

Technical Outcomes

The project successfully performed large-scale calculations of atomic nuclei and novel calculations of dense nucleonic matter present in neutron stars, which probe matter under conditions that cannot be created in any terrestrial experiments. The project results allowed us to place the most stringent constraints on the properties of neutron stars to date.

Publications

Journal Articles

Al-Mamun, M., A. W. Steiner, J. Nattila, J. Lange, R. O'Shaughnessy, I. Tews, S. Gandolfi, C. Heinke and S. Han. Combining Electromagnetic and Gravitational-Wave Constraints on Neutron-Star Masses and Radii. Submitted to *Physical Review Letters*. (LA-UR-20-26423)

*Capano, C. D., I. Tews, S. M. Brown, B. Margalit, S. De, S. Kumar, D. A. Brown, B. Krishnan and S. Reddy. Stringent constraints on neutron-star radii from multimessenger observations and nuclear theory. 2020. *Nature Astronomy*. **4** (6): 625-632. (LA-UR-19-28442 DOI: 10.1038/s41550-020-1014-6)

Dietrich, T., M. W. Coughlin, P. T. H. Pang, M. Bulla, J. Heinzel, L. Issa, I. Tews and S. Antier. New Constraints on the Supranuclear Equation of State and the Hubble Constant from Nuclear Physics--Multi-Messenger Astronomy. Submitted to *Science*. (LA-UR-20-21470)

Essick, R. C., P. Landry, A. Schwenk and I. Tews. A Detailed Examination of Astrophysical Constraints on the Symmetry Energy and the Neutron Skin of 208Pb with Minimal Modeling Assumptions. Submitted to *Physical Review C*. (LA-UR-21-21363)

Essick, R., P. Landry, A. Schwenk and I. Tews. Astrophysical Constraints on the Symmetry Energy and the Neutron Skin of 208-Pb with Minimal Modeling Assumptions. Submitted to *Physical Review Letters*. (LA-UR-21-20527)

Essick, R., P. Landry, I. Tews, S. Reddy and D. E. Holz. Direct Astrophysical Tests of Chiral Effective Field Theory. Submitted to *Physical Review C*. (LA-UR-20-22615)

*Lonardoni, D., I. Tews, S. Gandolfi and J. A. Carlson. Nuclear and neutron-star matter from local chiral interactions. 2020. *Physical Review Letters*. **2** (2): 022033. (LA-UR-19-32538 DOI: 10.1103/PhysRevResearch.2.022033)

Lonardoni, D. and I. Tews. Local chiral EFT potentials in nuclei and neutron matter: results and issues. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-22185 DOI: 10.22323/1.317.0100)

Pang, P. T., I. Tews, T. Dietrich, M. W. Coughlin, M. Bulla and C. Van Den Broeck. Nuclear Physics Multimessenger Astrophysics Constraints on the Neutron Star Equation of State: Adding NICER's PSR J0740+6620 Measurement. Submitted to *Astrophysical Journal*. (LA-UR-21-20534)

Pang, P. T., T. Dietrich, I. Tews and C. Van Den Broeck. Parameter estimation for strong phase transitions in supranuclear matter using gravitational-wave astronomy. Submitted to *Physical Review Research*. (LA-UR-20-24019)

*Piarulli, M. and I. Tews. Local Nucleon-Nucleon and Three-Nucleon Interactions Within Chiral Effective Field Theory. 2020. *Frontiers in Physics*. **7**: 245. (LA-UR-19-30461 DOI: 10.3389/fphy.2019.00245)

Schwenk, A. and I. Tews. Nukleare Zustandgleichung aus Gravitationswellenbeobachtungen (Nuclear equation of state from gravitational-wave observations). Submitted to *Physikjournal*. (LA-UR-21-20533)

*D. C. *. T. I. *. M. J. Somasundaram, R. *. and I. Tews. Constraints on the nuclear symmetry energy from asymmetric-matter calculations with chiral NN and 3N interactions. 2021. *Physical Review C*. **103** (4): 045803. (LA-UR-20-26894 DOI: 10.1103/PhysRevC.103.045803)

*Tews, I. Quantum Monte Carlo Methods for Astrophysical Applications. 2020. *Frontiers in Physics*. **8**. (LA-UR-19-32577 DOI: 10.3389/fphy.2020.00153)

*Tews, I. What can neutron stars reveal about the equation of state of dense matter?. *EPJ Web of Conferences*. **235**: 07002. (LA-UR-20-21735 DOI: 10.1051/epjconf/202023507002)

Tews, I., D. Lonardoni, K. Hebeler and L. Huth. Local chiral interactions up to next-to-next-to-leading order at larger cutoffs. Submitted to *Physical Review C.* (LA-UR-21-20525)

Tews, I., J. Margueron and S. Reddy. To which extend nuclear physics and GW170817 constrain the neutron star equation of state?. Submitted to *Proceedings for the CUSTIPEN XiAMEN Workshop*. (LA-UR-19-24461)

*Tews, I., P. T. H. Pang, T. Dietrich, M. W. Coughlin, S. Antier, M. Bulla, J. Heinzel and L. Issa. On the Nature of GW190814 and Its Impact on the Understanding of Supranuclear Matter. 2021. *The Astrophysical Journal Letters*. **908** (1): 6. (LA-UR-20-24959 DOI: 10.3847/2041-8213/abdaae)

*Tews, I., Z. Davoudi, A. Ekstrom, J. D. Holt and J. E. Lynn. New ideas in constraining nuclear forces. 2020. *Journal of Physics G: Nuclear and Particle Physics*. **47** (10): 103001. (LA-UR-19-32540 DOI: 10.1088/1361-6471/ab9079)

Reports

Dietrich, T. and I. Tews. Neutronensterne befl\xc3\xbcgeln Kosmologie und Kernphysik (Neutron stars spur cosmology and nuclear physics). *Spektrum der Wissenschaften (German popular science magazine)*. (LA-UR-21-20811)

Presentation Slides

Tews, I. Chiral effective field theory for the nuclear equation of state and neutron-star mergers. Presented at *2019 Fall Meeting of the APS Division of Nuclear Physics*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30581)

Tews, I. Chiral Effective Field Theory, Dense Nuclear Matter, and Neutron-Star Mergers. Presented at *JINA-INT Workshop Dense Matter & Neutron Star Mergers*, Seattle, Washington, United States, 2019-12-16 - 2019-12-18. (LA-UR-19-32539)

Tews, I. Stringent constraints on neutron-star radii from neutron-star mergers and chiral effective field theory. Presented at *Hirschegg 2020*, Hirschegg, Austria, 2020-01-13 - 2020-01-13. (LA-UR-20-20236)

Tews, I. Constraining the neutron-star equation of state and radius with chiral effective field theory and observations. Presented at *Ringberg conference*, Kreuth, Germany, 2020-01-13 - 2020-01-13. (LA-UR-20-20431)

Tews, I. From nuclei to neutron stars with local chiral interactions. Presented at *Theory Seminar at Washington University in St. Louis*, St. Louis, Missouri, United States, 2020-02-27 - 2020-02-27. (LA-UR-20-21840)

Tews, I. Constraining the neutron-star equation of state and radius with chiral effective field theory and observations. . (LA-UR-20-22616)

Tews, I. Constraining neutron-star matter with chiral effective field theory. Presented at *Second Nuclear and Particle Theory Meeting*, online, Missouri, United States, 2020-05-11 - 2020-05-12. (LA-UR-20-23507)

Tews, I. Nuclear-physics and multi-messenger constraints on the neutron-star equation of state. Presented at *Astrophysics/Gravity/Cosmology Seminar at University of Illinois at Urbana-Champaign (online)*, Los Alamos, New Mexico, United States, 2020-11-04 - 2020-11-04. (LA-UR-20-28940)

Tews, I. Dense-Matter Nuclear Theory. Presented at *JINA Horizons Virtual Meeting*, Los Alamos, New Mexico, United States, 2020-12-01 - 2020-12-04. (LA-UR-20-29793)

Tews, I. Nuclear-physics and multi-messenger constraints on the neutron-star equation of state. Presented at *IReNA online seminar*, Los Alamos, New Mexico, United States, 2020-12-11 - 2020-12-11. (LA-UR-20-30077)

Tews, I. NERSC Highlight slide. . (LA-UR-21-20568)

Tews, I. Quantum Monte Carlo Methods with chiral EFT Interactions as a consistent Approach to Nuclei and Neutron Stars. . (LA-UR-21-20814)

Tews, I. The nuclear equation of state in the era of neutron-star mergers. . (LA-UR-21-21910)

Tews, I. From nuclei to neutron stars: Combining nuclear physics and multimessenger observations. . (LA-UR-21-31977)

Tews, I. and D. Lonardoni. The nuclear equation of state at neutron-proton asymmetries (w21_eosafdmc). . (LA-UR-22-21625)

Posters

Tews, I. Matter and Nuclei at Neutron-rich Extremes. . (LA-UR-19-25831)

Tews, I. Neutron-Star Mergers as Probes for Nuclear Physics. Presented at *NUCLEI SciDAC PI meeting*, Rockville, Maryland, United States, 2019-07-15 - 2019-07-18. (LA-UR-19-26620)

Phase Diagrams and Conductivity in the Interiors of White Dwarf Stars

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20190624PRD2

Project Description

The extreme conditions found in stars and the wide range of multi-physics problems that must be solved to understand them overlaps considerably with the science of national security at the Laboratory. Astrophysics is a field where advanced models can be developed and tested and then applied to national security challenges. White dwarf stars in particular present exotic physical conditions not found in any other type of star and pose challenging problems to solve. The proposed work will address the calculation of material properties that are difficult to model, in particular the melting of mixtures and heat transport. These are two essential components for the modeling of white dwarfs. Our accurate plasma models and calculations will lead to better white dwarf models, with consequences for several fields of astrophysics. Moreover, the methods and tools we will develop are more generally applicable to the melting of pure substances and alloys, as well as heat transport in systems such as inertial confinement fusion. We anticipate that they will find fruitful applications in several areas of high energy density physics of relevance to national security, such as stockpile stewardship, where accurate material properties are a critical element to our theoretical understanding.

Technical Outcomes

All the proposed goals were completed successfully. The project was extended with the calculation of three additional melting curves to address interesting phenomena in white dwarfs of current interest to the astrophysics community. This expanded body of work enabled aclarification of the crystallization process in white dwarf stars. The new method developed to calculate the melting curve was successfully applied to four terrestrial metals. An extension to binary alloys was initiated.

Publications

Journal Articles

Bédard, A., P. Brassard, P. Bergeron and S. Blouin. On The Spectral Evolution of Hot White Dwarf Stars. II. Time-Dependent Simulations Of Element Transport In Evolving White Dwarfs With STELUM. Submitted to *Astrophysical Journal*. (LA-UR-21-28934)

Bergeron, P., F. Wesemael, G. Fontaine, R. Lamontagne, S. Demers, A. Bédard, M. Gingras, S. Blouin, M. J. Irwin and S. O. Kepler. Hot Degenerates in the MCT Survey. III. A Sample of White Dwarf Stars in the Southern Hemisphere. Submitted to *Astrophysical Journal*. (LA-UR-21-28033)

*Blouin, S. Magnesium abundances in cool metal-polluted white dwarfs. 2020. *Monthly Notices of the Royal Astronomical Society*. **496** (2): 1881-1890. (LA-UR-20-23364 DOI: 10.1093/mnras/staa1689)

*Blouin, S., J. Daligault, D. Saumon, A. Bedard and P. Brassard. Toward precision cosmochronology. 2020. *Astronomy & Astrophysics*. **640**: L11. (LA-UR-20-24795 DOI: 10.1051/0004-6361/202038879)

Blouin, S., J. O. Daligault and D. Saumon. 22Ne Phase Separation As A Solution To The Ultramassive White Dwarf Cooling Anomaly. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-22409)

*Blouin, S., N. R. Shaffer, D. Saumon and C. E. Starrett. New Conductive Opacities for White Dwarf Envelopes. 2020. *The Astrophysical Journal*. **899** (1): 46. (LA-UR-20-24054 DOI: 10.3847/1538-4357/ab9e75)

Blouin, S. and J. O. Daligault. Direct Evaluation of the Phase Diagrams of Dense Multicomponent Plasmas by Integration of the Clapeyron Equations. Submitted to *Physical Review E*. (LA-UR-21-20287)

*Blouin, S. and P. Dufour. The evolution of carbon-polluted white dwarfs at low effective temperatures. 2019. *Monthly Notices of the Royal Astronomical Society*. **490** (3): 4166-4174. (LA-UR-19-29175 DOI: 10.1093/mnras/stz2915)

Chandra, V., H. Hwang, N. L. Zakamska, S. Blouin, A. Swan, T. Marsh, K. J. Shen, B. T. Gänsicke, E. Petrosky, V. Dhillon, S. Littlefair and R. P. Ashley. Dynamic Circumstellar Debris around the SNIa Runaway LP 398-9. Submitted to *Astrophysical Journal*. (LA-UR-21-25924)

Harrison, J., A. Bonsor, M. Kama, A. Buchan and S. Blouin. Bayesian constraints on the origin and geology of exo-planetary material using a population of externally polluted white dwarfs. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-21-20941)

*Kaiser, B. C., J. C. Clemens, S. Blouin, P. Dufour, R. J. Hegedus, J. S. Reding and A. B\xc3\xa9dard. Lithium pollution of a white dwarf records the accretion of an extrasolar planetesimal. 2021. *Science*. **371** (6525): 168-172. (LA-UR-20-24419 DOI: 10.1126/science.abd1714)

*Kilic, M., P. Bergeron, A. Kosakowski, W. R. Brown, M. A. Ag \xc3\xbceros and S. Blouin. The 100 pc White Dwarf Sample in the SDSS Footprint. 2020. *The Astrophysical Journal*. **898** (1): 84. (LA-UR-20-23514 DOI: 10.3847/1538-4357/ab9b8d)

*Kilic, M., P. Bergeron, S. Blouin and A. B\xc3\xa9dard. The most massive white dwarfs in the solar neighbourhood. 2021. *Monthly Notices of the Royal Astronomical Society*. **503** (4): 5397-5408. (LA-UR-21-20639 DOI: 10.1093/mnras/stab767)

Klein, B., A. Doyle, B. Zuckerman, P. Dufour, S. Blouin, C. Melis, A. Weinberger and E. Young. Discovery of Beryllium in White Dwarfs Polluted by Accreted Planetesimals. Submitted to *Astrophysical Journal*. (LA-UR-20-29805)

*Klein, B., S. Blouin, D. Romani, B. Zuckerman, C. Melis, S. Xu, P. Dufour, C. Genest-Beaulieu, A. Bedard and M. Jura. Atmospheric Temperature Inversions and He i 5876 Core Profile Structure in White Dwarfs. 2020. *The Astrophysical Journal*. **900** (1): 2. (LA-UR-20-22642 DOI: 10.3847/1538-4357/ab9b24)

*Lam, M. C., N. C. Hambly, N. Lodieu, S. Blouin, E. J. Harvey, R. J. Smith, M. C. Galvez-Ortiz and Z. H. Zhang. First discovery of an ultra-cool white dwarf benchmark in common proper motion with an M dwarf. 2020. *Monthly Notices of the Royal Astronomical Society*. **493** (4): 6001-6010. (LA-UR-19-31660 DOI: 10.1093/mnras/staa584)

Saumon, D., S. Blouin and P. Tremblay. Current challenges in the physics of white dwarf stars. Submitted to *Physics Reports*. (LA-UR-22-22094)

Vanderbosch, Z., S. Rappaport, J. A. Guidry, B. L. Gary, S. Blouin, T. G. Kaye, A. Weiberger, C. Melis, B. Klein, B. Zuckerman, A. Vanderburg, J. Hermes, R. J. Hegedus, M. R. Burleigh, R. Sefako and T. M. Heintz. ZTF J0328-1219: A Third Case of Transiting Planetary Debris around a White Dwarf. Submitted to *Astrophysical Journal*. (LA-UR-21-21884)

*Vanderburg, A., S. A. Rappaport, S. Xu, I. Crossfield, J. C. Becker, B. Gary, F. Murgas, S. Blouin and l. i. t. p. And 53 other non-LANL authors. A giant planet candidate transiting a white dwarf. 2020. *Nature*. **585** (7825): 363-367. (LA-UR-20-21720 DOI: 10.1038/s41586-020-2713-y)

Xu, S., H. Diamond-Lowe, R. J. MacDonald, A. Vanderburg, S. Blouin, P. Dufour, P. Gao, L. Kreidberg, S. K. Leggett, A. W. Mann, C. V. Morley, A. Stephens, C. E. O'Connor, P. C. Thao and N. K. Lewis. Gemini/GMOS Transmission Spectroscopy of the Grazing Planet Candidate WD 1856+534 b. 2021. *The Astronomical Journal*. **162** (6): 296. (LA-UR-21-25312 DOI: 10.3847/1538-3881/ac2d26)

Conference Papers

Blouin, S. and P. Dufour. The Spectral Evolution of Cool White Dwarfs. Presented at *IAU Symposium 357: White Dwarfs as probes of fundamental physics and tracers of planetary, stellar & galactic evolution*. (Hilo, Hawaii, United States, 2019-10-21 - 2019-10-25). (LA-UR-19-31433)

Presentation Slides

Blouin, S. The spectral evolution of cool white dwarfs. Presented at *International Astronomical Union Symposium 357: White Dwarfs as probes of fundamental physics and tracers of planetary, stellar & galactic evolution*, Hilo, Hawaii, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-29925)

Blouin, S. When The Fit Is Just Right: Improved Cool White Dwarf Atmosphere Models. Presented at *235th Meeting of the American Astronomical Society*, Honolulu, Hawaii, United States, 2020-01-04 - 2020-01-08. (LA-UR-19-32098)

Blouin, S. Cool white dwarf atmospheres: From condensed matter physics to stellar archeology. Presented at *Annual Meeting of the Canadian Astronomical Society*, Online meeting, Canada, 2020-05-25 - 2020-05-28. (LA-UR-20-23444)

Blouin, S. Cool white dwarf atmospheres: From condensed matter physics to stellar archeology. Presented at *Annual Meeting of the Canadian Astronomical Society*, Online meeting, Canada, 2020-05-25 - 2020-05-28. (LA-UR-20-23636)

Blouin, S. Cool white dwarf atmospheres: A transparent window into the past. Presented at *Space Telescope Science Institute Seminar (remote)*, Baltimore, Maryland, United States, 2020-09-03 - 2020-09-03. (LA-UR-20-26543)

Blouin, S. Cool white dwarf atmospheres: A transparent window into the past. Presented at *Space Telescope Science Institute Seminar (remote)*, Baltimore, Maryland, United States, 2020-09-03 - 2020-09-03. (LA-UR-20-27315)

Blouin, S. Calculating Melting Curves for Crystallizing Stars. Presented at *XCP Seminar*, Los Alamos, New Mexico, United States, 2020-11-05 - 2020-11-05. (LA-UR-20-28803)

Blouin, S., J. O. Daligault, N. R. Shaffer, D. Saumon, A. B \xc3\xa9dard, P. Brassard and C. E. Starrett. New Melting Curves and Conductive Opacities for White Dwarfs. Presented at *237th Meeting of the American Astronomical Society*, Online, New Mexico, United States, 2021-01-11 - 2021-01-15. (LA-UR-21-20081)

Blouin, S., J. O. Daligault and D. Saumon. A New C/O Plasma Melting Curve For White Dwarf Core Crystallization. Presented at *62nd Annual Meeting of the APS Division of Plasma Physics*, Online, New Mexico, United States, 2020-11-09 - 2020-11-13. (LA-UR-20-28917)

The Ultimate Search for the Color Glass Condensate

Renaud Boussarie
20200683PRD1

Project Description

The internal structure and dynamics of protons, neutrons and nuclei is one of the greatest scientific puzzles of our time. The simple image of the proton as three quarks bound together by the strong interaction via exchange of gluons is rendered immensely complicated by the fact that gluons themselves interact with each other. Thus, the origin of the proton spin is still not known, nor do we yet understand the origin of its mass and the mass of visible matter. One of the big theoretical discoveries of the late 20th century is that at extremely high energies nucleons and nuclei that make up our universe exhibit remarkable simplicity and evolve into a dense saturated state of gluons. This new state of matter, known as the Color Glass Condensate (CGC), may hold the answers to those puzzles. The Electron-Ion Collider (EIC), the number one priority for a new facility for the Department of Energy, will be a perfect microscope into the content of hadrons and the ideal machine to discover gluon saturation and revolutionize our understanding of matter at all length scales. This research will develop the tools needed to discover the Color Glass Condensate and enhance EIC science.

Technical Outcomes

The project completed important work on transverse momentum physics and the connection to the Color Glass Condensate. Progress was made toward understanding the production of jets at the Electron-Ion Collider (EIC) in the gluon saturation regime.

Publications

Books/Chapters

Lee, C., I. M. Vitev, R. Boussarie, J. W. Qiu, I. W. Stewart, T. Mehen, M. Burkardt, M. Constantinou, W. Detmold, M. Ebert, M. Engelhardt, S. Fleming, L. Gamberg, X. Ji, Z. B. Kang, K. F. Liu, S. Liuti, A. Metz, J. Negele, D. Pitonyak, A. Prokudin, A. Rajan, M. Schlegel, P. Shanahan, P. Schweitzer, A. Tarasov, R. Venugopalan, F. Yuan and Y. Zhao. TMD Handbook: A modern introduction to the physics of Transverse Momentum Dependent distributions. (LA-UR-21-20798)

Precision Nuclear Tomography at the Electron-Ion Collider

Ivan Vitev
20200773PRD4

Project Description

Our United States strategy in nuclear science calls for leadership role at the future Electron-Ion Collider (EIC). There is ongoing dedicated experimental work to design a detector that can measure heavy particles and jets in the proton and nucleus going direction. Theoretical advances to guide such design and to shape the nuclear tomography pillar of EIC science are both critical and timely. This research project will lead to a leap in the precision of theoretical calculations for the most pertinent experimental observables and enable their use to extract the transport properties of large nuclei. Quantitative description of subatomic particle shower formation in dense environments can give valuable insights for areas of applied nuclear research at Los Alamos National Lab.

Technical Outcomes

This project met its goals and advanced the physics of heavy flavor mesons and jet. It produced novel insights into the process of hadronization and the use of heavy flavor-tagged jets for nuclear tomography. The focus was specifically at the future Electron-Ion Collider. The team developed expertise that positions Los Alamos to be leaders at the heavy flavor program at the Electron-Ion Collider.

Implementing a Novel Ultrasonic Filtration Technology to Eliminate Hydroxide Precipitation Bottlenecks at TA-55

James Coons
20210538MFR

Project Description

The ultimate goal of this endeavor is a functional revolutionary hydroxide precipitation process which utilizes a novel separation technology called ultrasonic filtration. This disruptive technology would replace a physical membrane with an ultrasonic field that retains solid particles while allowing the particle-free media to pass through. By eliminating the physical barrier, solids removal occurs much faster in a closed, continuous operation. Ultrasonic filtration will eliminate the separation bottle necks at Technical Area-55, dramatically reduce dose and physical demands on operators, and improve the caustic glovebox atmospheres that contribute to equipment corrosion and limited lifetimes. This groundbreaking hydroxide precipitation process builds upon existing ultrasonic separations technology, but substantial work is required to produce a functional system in a flow-through configuration operational in gloveboxes in nuclear facilities. This Phase 1 project aims to understand performance-bounding properties including the settling behavior of surrogate hydroxide particles and aggregates, and assess the performance of ultrasonic filtration over a range of scales. These baseline tests are essential for the Phase 2 study focusing on overcoming fundamental impediments for improved prototype system performance.

Publications

Presentation Slides

Roman, A. R., J. E. Coons and A. J. Parkison. Ultrasonic Filtration: A Revolutionary Technology for Hydroxide Precipitation. Presented at *Engineering Week Webex Meeting*, Los Alamos, New Mexico, United States, 2021-02-22 - 2021-02-24. (LA-UR-21-21714)

Megavolt generator for multiple-pulse hydrotesting

Nicola Winch
20210540MFR

Project Description

Los Alamos leads the world in multiple-pulse radiography but this can only be done at very large accelerator facilities such as the Dual-Axis Radiographic Hydrodynamic Test (DARHT) Facility and Los Alamos Neutron Science Center (LANSCE). This is very expensive, and a lot of types of shots would benefit from smaller scale, low cost, portable, multiple pulse radiography. PHOENIX (Portable, High efficiency, Optimal ENergy, Imaging X-rays) can return multiple-pulse radiography to the small scale firing sites. Current x-ray generators at small scale firing sites are 1960s Febetrons, which have both safety and reliability issues and are not multiple pulsed machines. PHOENIX will benefit the weapons engineering mission by providing portable multiple pulse radiography to the small scale firing sites, a Los Alamos Goal since the Manhattan Project. A modified version would benefit the global security mission by providing a man portable, low power, megavolt source to nuclear emergency response teams.

Modeling Late-Time Electromagnetic Pulse and Its Disturbed Atmospheric Environment

Christopher Jeffery
20190541MFR

Project Description

A high-altitude nuclear explosion (HANE) can significantly disturb the Earth's upper atmosphere, resulting in the generation of a late-time electromagnetic pulse (EMP) and an environment that negatively affects radio wave propagation across a broad range of frequencies. We are developing a computer model that will allow us to simulate the disturbance of the atmosphere by a HANE, the generation of EMP in this disturbed atmosphere, and the subsequent development of an environment that could greatly impair the efficacy of radio communications.

Technical Outcomes

This project advanced Los Alamos' High Altitude Nuclear Explosion "E3B" (Heave) modeling capability. The team coupled unique Laboratory Electromagnetic and high-altitude nuclear event/explosion (HANE) codes with Naval Research Lab's state-of-the-art ionospheric modeling code, "SAMI3." The team used Los Alamos codes from X-division to model HANE, then input those fields into SAMI-3. Deficiencies with SAMI-3 chemistry and numerical performance were found, which led the team to implement some of the SAMI-3 physics into the Los Alamos GeoRad code.

Publications

Reports

M. Jeffery, C. A. Introducing GeoRad: A Variable-Resolution EMP Solver on an Unstructured Voronoi Tessellation. Unpublished report. (LA-UR-19-29953)

Presentation Slides

M. Jeffery, C. A., E. H. Lay, K. R. Costigan, W. P. Even, E. M. Nelson, H. E. Morris and M. J. Peterson. The Nuclear-Disturbed Environment: E3, HF/VHF Absorption & the Monitoring Potential of Our SNDD EMP System. Presented at *SGSIE 2020*, Los Alamos, New Mexico, United States, 2020-11-02 - 2020-11-06. (LA-CP-20-20658)

Posters

M. Jeffery, C. A., E. H. Lay, K. R. Costigan, W. P. Even, H. E. Morris and M. Worstell. Modeling High-Energy Disturbances in GeoRad: Impacts on D-Region Chemistry and Knapp's Three Species Model. Presented at *Fall AGU*, Online, New Mexico, United States, 2020-12-15 - 2020-12-15. (LA-UR-20-30243)

M. Jeffery, C. A., K. R. Costigan, E. H. Lay and H. E. Morris. Test of a Multigrid Method for Ionospheric Temperature Modeling. Presented at *Fall AGU*, San Francisco, California, United States, 2019-12-13 - 2019-12-13. (LA-UR-19-32621)

Detector Response Toolkit for Nuclear Emergency Response

Madison Andrews
20210573MFR

Project Description

This project would provide a high-fidelity 3-Dimensional detector response link in the nuclear emergency response chain which harnesses the powerful radiation transport and measurement analysis tools already developed by Los Alamos National Laboratory (LANL). This project would generate methodology, tools, and techniques which also would be utilized outside of Nuclear Emergency Response (NER) and would potentially provide a basis for systematic improvements for work done in: diagnostics, detector development, nuclear safeguards and nonproliferation.

Technical Outcomes

This project significantly expanded nuclear instrumentation simulation capabilities of the Detector Response Function Toolkit code to include semiconductor and gas-type detectors with many environmental (temperature, detector damage) and instrument setting (quench gas, anode size, applied voltage) variables. Additional features developed include electronics modules which facilitate an accurate simulation of applied voltage, pile-up, and damage effects, all of which are highly relevant to Nuclear Emergency response (NER) scenarios and not available, or simulated with low fidelity in current NER codes.

Publications

Conference Papers

Andrews, M. T., A. C. Madden, D. R. Mayo and S. F. Woldegiorgis. Preliminary Helium-3 Detector Response Capabilities in DRiFT. Presented at *ICRS 14/RPSD 2021*. (Seattle, Washington, United States, 2021-09-12 - 2021-09-16). (LA-UR-21-21199)

Presentation Slides

Andrews, M. T. DRiFT - Detector Response Function Toolkit Organic Scintillator and Gas Detector Capability Overview. . (LA-UR-21-30479)

Andrews, M. T., S. F. Woldegiorgis, D. R. Mayo and A. Sood. Gas and Semiconductor Capability Development in DRiFT: Description, Demonstration, and Discussion. Presented at *Discussion with LANL Program Manager*, Los Alamos, New Mexico, United States, 2021-05-28 - 2021-05-28. (LA-UR-21-25046)

Andrews, M. T., S. F. Woldegiorgis and D. R. Mayo. MFR Mid Year Project Visit - Detector Response Toolkit for Nuclear Emergency Response. Presented at *MFR Mid-year review*, Webex, New Mexico, United States, 2021-03-16 - 2021-03-16. (LA-UR-21-22433)

Nuclear Material Control and Accounting (NMC&A)/In-line Monitoring Capability (ILM)

Rollin Lakis
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Project Description

The primary goal of the In-Line Monitoring Project is to enhance manufacturing agility and efficiency in a nuclear material production environment, and improve nuclear security by modernizing, streamlining and optimizing quantitative nuclear material measurements and nuclear material control and accounting (NMC&A). Increased confidence will be achieved through the use of modern data analysis and statistical approaches coupled with optimized nondestructive assay (NDA) instruments, applied in-line or at-line in nuclear production environments.

Publications

Conference Papers

Ren, C. X., E. M. Casleton, S. E. Sarnoski, T. J. I. Stockman, A. N. Skurikhin, B. P. Weaver, V. Henzl, A. Favalli and R. E. Lakis. Source term estimation via combined sparse convex optimization and maximum liklihood extimation for nuclear material accounting. Presented at *INMM*. (Virtual, Austria, 2021-08-23 - 2021-09-01). (LA-UR-21-27798)

Sarnoski, S. E., T. J. I. Stockman, E. M. Casleton, C. W. Graham, V. Henzl, M. Iliev, P. M. Mendoza, M. R. Newell, C. D. Rael, C. X. Ren, A. N. Skurikhin, J. Stinnett, D. T. Vo, B. P. Weaver, R. Weinmann-Smith, A. Favalli and R. E. Lakis. Analysis of in-line plutonium mass measurements, in a dynamic background environment, for nuclear material control and accounting in nuclear fuel cycle facilities. Presented at *INMM 2021 Annual Meeting*. (Virtual, New Mexico, United States, 2021-08-23 - 2021-08-26). (LA-UR-21-27969)

Presentation Slides

Cattaneo, A., E. M. Casleton, C. Chavez, H. H. Erpenbeck, A. Favalli, W. H. Geist, V. Henzl, D. C. Henzlova, M. Iliev, K. E. Koehler, R. E. Lakis, P. M. Mendoza, M. R. Newell, C. D. Rael, C. X. Ren, S. E. Sarnoski, A. N. Skurikhin, J. Stinnett, T. J. I. Stockman, D. T. Vo, B. P. Weaver and R. Weinmann-Smith. DYMAC LDRD Review. . (LA-UR-21-25652)

Henzl, V., K. E. Koehler, P. M. Mendoza, S. E. Sarnoski and B. P. Weaver. Key Measurement Points Optimization. Presented at *INMM/ESARDA 2021*, Vienna, Austria, 2021-08-23 - 2021-08-23. (LA-UR-21-28602)

Hitson, S. C., V. Henzl, K. E. Koehler, P. M. Mendoza and S. E. Sarnoski. Key Measurement Points Optimization Project. Presented at *LANL Annual Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27495)

Lakis, R. E. In Line Monitoring / Dynamic Material Control (DYMAC): Advanced Non Destructive Analysis (NDA) and Real-Time Special Nuclear Materials (SNM) Inventory. . (LA-UR-21-28431)

Ren, C. X., E. M. Casleton, S. E. Sarnoski, T. J. I. Stockman, A. N. Skurikhin, B. P. Weaver, V. Henzl, A. Favalli and R. E. Lakis. Source term estimation via combined sparse convex optimization and maximum likelihood estimation for nuclear material accounting. Presented at *INMM*, Vienna, Austria, 2021-08-23 - 2021-08-23. (LA-UR-21-28019)

I. Stockman, T. J. Facility scale in-situ source localization and assay via a sparse 3He neutron detector array: enhancing nuclear material control and accounting in nuclear fuel cycle facilities. Presented at *INMM 2021*, Virtual, Austria, 2021-08-23 - 2021-08-25. (LA-UR-21-28490)

Posters

Sarnoski, S. E. and T. J. I. Stockman. Analysis of in-line plutonium mass measurements, in a dynamic background environment, for nuclear material control and accounting in nuclear fuel cycle facilities. Presented at *INMM Annual Meeting*, Virtual, New Mexico, United States, 2021-08-23 - 2021-08-23. (LA-UR-21-28134)

Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors

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Project Description

Innovative nuclear reactor designs are currently being proposed to increase efficiency and economic viability of nuclear energy production. Microreactors are one example of a portable reactor concept that can provide power in remote environments. In support of these designs, moderated materials such as yttrium hydride provide reductions in the size requirements of the system. Understanding of hydrogen dynamics, i.e. the behavior of hydrogen atoms in materials as a function of temperature and hydrogen concentration, is of paramount importance for applications that assess material behavior (e.g. corrosion) of these advanced moderators. The combination of experimental results and advanced multi-physics simulation tools from this project will further our understanding and ultimately provide predictive capabilities of hydrogen behavior in a nuclear reactor. These capabilities can be applied to other hydrogen-related problems after the end of this project. A high fidelity hydrogen mapping capability will be developed at LANSCE, and a new multi-physics framework for a range of reactor design analysis will be generated.

Technical Outcomes

This project significantly advanced Los Alamos' ability to predict performance of moderator material with both experimental and theoretical research, and capabilities developed through this project will be able to be applied to a wide range of future systems and applications. The team observed the redistribution of hydrogen at temperatures above 780°Celsius in yttrium hydride material, developed a comprehensive framework for predicting yttrium hydride behavior, and benchmarked our predictions with experimental methods.

Publications

Journal Articles

Mehta, V. K., J. C. Armstrong, V. R. Dasari and D. Kotlyar. Capturing Multiphysics Effects in Hydride Moderated Microreactors using MCNP and ABAQUS. Submitted to *Applied Sciences*. (LA-UR-21-20451)

*Mehta, V. K., S. C. Vogel, A. P. Shivprasad, E. P. Luther, D. A. Andersson, D. V. Rao, D. Kotlyar, B. Clausen and M. W. Cooper. A density functional theory and neutron diffraction study of the ambient condition properties of sub-stoichiometric yttrium hydride. 2021. *Journal of Nuclear Materials*. **547**: 152837. (LA-UR-20-24029 DOI: 10.1016/j.jnucmat.2021.152837)

Mehta, V. K., S. C. Vogel, M. W. D. Cooper and D. Kotlyar. Direct Observation of Bredig Transition in Yttrium Hydride (YH2-x). Submitted to *Physical Review Letters*. (LA-UR-20-26447)

Mehta, V. K., S. C. Vogel, M. W. D. Cooper and D. Kotlyar. A Modeling and Neutron Diffraction Study of the High Temperature Properties of Sub-Stoichiometric Yttrium Hydride for Novel Moderator Applications. Submitted to *Metals*. (LA-UR-21-23936)

Mehta, V. K., S. C. Vogel, R. B. Wilkerson, D. Kotlyar, M. W. D. Cooper and V. R. Dasari. Evaluation of Yttrium Hydride (\xce\xb4-YH2-x) Thermal Neutron Scattering Laws and Thermophysical Properties. Submitted to *Nuclear Science and Engineering*. (LA-UR-20-26691)

*Shivprasad, A. P., S. C. Vogel, V. K. Mehta, M. W. D. Cooper, T. A. Saleh, J. T. White, J. R. Wermer, E. P. Luther and H. R. Trellue. Thermophysical properties of high-density, sintered monoliths of yttrium dihydride in the range 373–773\xc2\xa0K. 2021. *Journal of Alloys and Compounds*. **850**: 156303. (LA-UR-20-23935 DOI: 10.1016/j.jallcom.2020.156303)

Trellue, H. R., A. M. Long, E. P. Luther, D. T. Carver and V. K. Mehta. Effects of Hydrogen Redistribution at High Temperatures in Yttrium Hydride Moderator Material. Submitted to *Journal of Materials*. (LA-UR-21-24178)

Conference Papers

Wilkerson, R. B., G. W. Mckinney, C. J. Josey, M. e. Blood, J. D. Galloway, J. C. Armstrong and H. R. Trellue. Advances in MCNP for Reactor Calculations. Presented at *American*

Nuclear Society Annual Meeting. (Phoenix, Arizona, United States, 2020-06-07 - 2020-06-11). (LA-UR-20-20505)

Reports

Armstrong, J. C. and K. C. Kelley. Generating MCNP Input Files for Unstructured Mesh Geometries. Unpublished report. (LA-UR-20-27139)

D. Cooper, M. W. and V. K. Mehta. Modeling of Moderator Materials for Micro-reactors. Unpublished report. (LA-UR-21-23720)

Mehta, V. K. Investigating the Response of Yttrium Hydride Moderator Due to Changes in Stoichiometry and Temperature. Unpublished report. (LA-UR-20-23082)

Mehta, V. K. INVESTIGATING THE RESPONSE OF YTTRIUM HYDRIDE MODERATOR DUE TO CHANGES IN STOICHIOMETRY AND TEMPERATURE. Unpublished report. (LA-UR-20-29128)

Mehta, V. K. and J. C. Armstrong. Processing MCNP Elemental Edit Outputs. Unpublished report. (LA-UR-20-24025)

Trellue, H. R., S. C. Vogel, A. M. Long, V. K. Mehta, J. C. Armstrong, G. W. Mckinney, A. P. Shivprasad, E. P. Luther, M. W. D. Cooper, R. B. Wilkerson, J. E. Payne, D. T. Carver, M. E. Rising, J. S. Bull and J. A. Kulesza. Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors. Unpublished report. (LA-UR-21-24964)

Wilkerson, R. B., G. McKinney, M. E. Rising and J. A. Kulesza. MCNP Reactor Multigroup Tally Options Verification. Unpublished report. (LA-UR-20-27819)

Presentation Slides

Armstrong, J. C. and M. E. Rising. MCNP Code Modernization & Code Improvement for Microreactor Multiphysics Calculations. . (LA-UR-20-23568)

D. Cooper, M. W. and V. K. Mehta. Modeling of moderator materials for micro-reactors. . (LA-UR-21-23722)

Mehta, V. K., J. C. Armstrong and V. R. Dasari. MCNP and ABAQUS based Reactor Multiphysics (MARM). Presented at *MCNP Symposium*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-12. (LA-UR-21-26454)

Shivprasad, A. P., D. M. Frazer, E. P. Luther, S. C. Vogel, A. M. Long, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer, H. R. Trellue and V. R. Dasari. Properties of sintered yttrium dihydride for nuclear reactor moderator applications. Presented at *INTERNATIONAL CONFERENCE ON PROCESSING & MANUFACTURING OF ADVANCED MATERIALS (THERMEC 2021)*, Online, New Mexico, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-21862)

Shivprasad, A. P., E. P. Luther, A. M. Long, T. E. Cutler, T. J. Grove, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R.

Wermer and H. R. Trellue. High temperature moderator material for Microreactors. . (LA-UR-20-21710)

Shivprasad, A. P., E. P. Luther, S. C. Vogel, A. M. Long, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer, H. R. Trellue and V. R. Dasari. Thermophysical properties of sintered yttrium dihydride. Presented at *MS&T 2020*, Online, New Mexico, United States, 2020-11-02 - 2020-11-02. (LA-UR-20-28532)

Shivprasad, A. P., E. P. Luther, S. C. Vogel, T. E. Cutler, V. K. Mehta, M. W. D. Cooper, J. T. White, T. A. Saleh, J. R. Wermer, H. R. Trellue and A. M. Long. High temperature moderator capabilities at LANL. Presented at *NASA Moderator TIM*, Los Alamos, New Mexico, United States, 2020-10-15 - 2020-10-15. (LA-UR-20-28214)

Shivprasad, A. P., T. A. Saleh, C. A. Taylor, V. K. Mehta, M. W. D. Cooper, S. C. Vogel, A. M. Long, T. J. Nizolek, E. P. Luther, J. R. Wermer, H. R. Trellue, V. R. Dasari and W. T. Buttler. Metal hydride moderator development at LANL. Presented at *Materials in Nuclear Energy Systems*, Pittsburgh, New Mexico, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-31070)

Shivprasad, A. P., V. K. Mehta, M. W. D. Cooper, T. A. Saleh, J. T. White, J. R. Wermer, E. P. Luther and H. R. Trellue. Thermophysical properties of yttrium dihydride. Presented at *44th International Conference and Expo on Advanced Ceramics and Composites (ICACC 2020)*, Daytona Beach, Florida, United States, 2020-01-26 - 2020-01-26. (LA-UR-20-20540)

Trellue, H. R., S. C. Vogel, A. M. Long, J. C. Armstrong, V. K. Mehta, M. W. D. Cooper, A. P. Shivprasad, E. P. Luther and M. e. Blood. Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors - FY19. . (LA-UR-19-30226)

Trellue, H. R., S. C. Vogel, A. M. Long, V. K. Mehta, J. C. Armstrong, G. W. Mckinney, A. P. Shivprasad, E. P. Luther, J. E. Payne, M. W. D. Cooper, D. T. Carver, R. B. Wilkerson, J. R. Wermer and J. S. Bull. Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors. . (LA-UR-20-22974)

Trellue, H. R. and M. J. Monreal. Advanced Reactor Technological Enhancements. . (LA-UR-21-25473)

Posters

Mehta, V. K. Computational Physics Aspects of Metal Hydride Moderators. . (LA-UR-21-25635)

Other

Mehta, V. K. Releasing Yttrium Hydride Thermal Scattering Laws (TSLs) for Cross Section Evaluation Working Group (CSEWG) peer review. Dataset. (LA-UR-21-21948)

Cryogenically Cooled Particle Accelerators for Transformative Improvement

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20210691DI

Project Description

This project gives critical information that will be necessary to construct a compact high-energy particle accelerators operated at a very cold temperature. This accelerator will provide National Nuclear Security Administration (NNSA) with the capability of penetrating radiography of dense imploding systems required for the stockpile stewardship program. High-energy electron radiography may be a transformative technology for future dynamic materials studies. The compact high-energy accelerators can also be used for active interrogation of material to search for special nuclear material at border crossings and in space to interrogate the boundary layers in the ionosphere.

Technical Outcomes

The project was successfully executed. The team developed techniques to cool down accelerator structures down to <7 kelvin (K) vs. required <40 K, and measured temperature dependences of resonant frequency and surface resistance that was very close to theoretical values. The team also conducted thermal and multi-physics simulations and thermal simulation results were compared with experimental results. The multi-physics simulation results gave important insights into the future high-power tests.

Publications

Conference Papers

Pizzol, P., J. W. I. Lewellen, E. R. Olivas, E. I. Simakov and T. Tajima. Design, construction and tests of the cooling system with a cryocooler for cavity testing.. Presented at *IPAC 2021*. (Campinas, Brazil, 2021-05-24 - 2021-05-28). (LA-UR-21-24677)

Presentation Slides

Pizzol, P., J. W. I. Lewellen, E. R. Olivas, E. I. Simakov and T. Tajima. Design, construction and tests of the cooling system with a cryocooler for cavity testing. Presented at *IPAC 2021*, Campinas, Brazil, 2021-05-24 - 2021-05-28. (LA-UR-21-24676)

Science of Signatures

Hyperspectral Xray Imaging (HXI): Nanochemical Analysis of Actinide and Explosive Materials (U)

Mark Croce
20190002DR

Project Description

Small particles containing uranium compounds can come from almost anywhere in the nuclear fuel cycle or on the road to making a nuclear bomb. Characterization of their detailed chemical form is needed to understand potential material origins, history, and environmental fate. The International Atomic Energy Agency (IAEA) and the United States Air Force Technical Applications Center (AFTAC) have stated that chemical speciation, especially uranium oxidation state, is very important for small particles. Outside of the brightest light sources, mammoth synchrotron laboratories, there is no x-ray chemical analysis method that provides a comprehensive determination of actinide (uranium, plutonium) chemical form and the spatial resolution needed to study microscopic samples with nanoscale heterogeneity. We will develop the first comprehensive chemical analysis capability in a regular laboratory for such particles by combining ultra-high-resolution microcalorimeter x-ray detectors with a scanning electron microscope, and interpreting the data with advanced theoretical methods. There are few institutions in a position to fully implement this technology. Only Los Alamos is in a position to develop this technology for laboratory-based materials analysis, and only Los Alamos has a nuclear materials mandate. This project will create a new analytical capability to support national security priorities.

Publications

Journal Articles

Carpenter, M. H., B. Stein, K. E. Koehler, C. J. Fontes, C. M. Smith, G. L. Wagner, Z. K. Baker, M. L. Handley, M. W. Rabin, P. Yang, E. R. Batista, D. G. McNeel, K. A. Schreiber, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. S. Swetz, D. R. Schmidt, D. T. Becker, J. A. B. Mates, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels and M. P. Croce. Hyperspectral X-ray Imaging: Progress Towards Chemical Analysis in the SEM. Submitted to *IEEE Transactions on Applied Superconductivity*. (LA-UR-20-28609)

Carpenter, M. H., M. P. Croce, Z. K. Baker, E. R. Batista, M. P. Caffrey, C. J. Fontes, K. E. Koehler, S. E. Kossmann, K. G. McIntosh, M. W. Rabin, B. W. Renck, G. L. Wagner, M. P. Wilkerson, P. Yang, M. D. Yoho, J. N. Ullom, D. A. Bennett, G. C. O'Neil, C. D. Reintsema, D. R. Schmidt, G. C. Hilton, D. S. Swetz, D. T. Becker, J. D. Gard, J. Imrek, J. A. B. Mates, K. M. Morgan, D. Yan, A. L. Wessels, R. H. Cantor, J. A. Hall and D. T. Carver. Hyperspectral X-ray Imaging with TES Detectors for Nanoscale Chemical Speciation Mapping. 2020. *Journal of Low Temperature Physics*. **200** (5-6): 437-444. (LA-UR-19-27148 DOI: 10.1007/s10909-020-02456-9)

Li, J., L. Xu, M. Garcia-Fernandez, A. Nag, H. C. Robarts, A. C. Walters, X. Liu, J. Zhou, K. Wohlfeld, J. van den Brink, H. Ding and K. Zhou. Unraveling the Orbital Physics in a Canonical Orbital System KCuF3. 2021. *Physical Review Letters*. **126** (10): 106401. (LA-UR-20-27035 DOI: 10.1103/PhysRevLett.126.106401)

Presentation Slides

Batista, E. R., P. Yang and L. Xu. Prediction of XES spectra for molecular systems. Presented at *LDRD Review*, Los Alamos, New Hampshire, United States, 2020-08-11 - 2020-08-11. (LA-UR-20-26148)

Carpenter, M. H., M. P. Croce, C. M. Smith and K. E. Koehler. High-Resolution Chemical-State Mapping and Analysis for Nuclear Safeguards with Microcalorimeter SEM-EDS. Presented at *Microscopy and Microanalysis 2020*, Virtual, New Mexico, United States, 2020-08-02 - 2020-08-07. (LA-UR-20-25285)

Croce, M. P. New Analytical Capabilities with Microcalorimeters. . (LA-UR-19-27141)

Croce, M. P. Microcalorimeter Technology for Enhanced Safeguards Capabilities. Presented at *INMM-ESARDA-INMMJ Workshop*, Tokyo, Japan, 2019-10-07 - 2019-10-07. (LA-UR-19-29984)

Croce, M. P. IAEA Sample Results and Microcalorimeter Capabilities. . (LA-UR-19-30668)

Croce, M. P. Non-Destructive Evaluation Capabilities with Calorimetry and Microcalorimetry. Presented at *2019 Pit CEPPC*, Los Alamos, New Mexico, United States, 2019-06-19 - 2019-06-19. (LA-UR-19-30824)

Croce, M. P. LANL LTD Projects. . (LA-UR-19-31710)

Croce, M. P., M. H. Carpenter, K. E. Koehler, D. G. McNeel, K. A. Schreiber, C. M. Smith and S. L. Weidenbenner. Low-Temperature Detectors for High-Precision Measurements. . (LA-UR-21-24545)

Koehler, K. E. Microcalorimeters: A Bright, Bold Future. Presented at *SeeLANL*, Los Alamos, New Mexico, United States, 2020-01-13 - 2020-01-13. (LA-UR-20-20224)

Koehler, K. E. Microcalorimeters: A Bright, Bold Future. . (LA-UR-21-23649)

Koehler, K. E. and C. J. Fontes. Spectral Calculations of X-ray Emission for Microcalorimeter Measurements: Theoretical basis for small mystery peaks in experimental x-ray measurements. Presented at *MetroMMC Stakeholder Meeting*, Saclay, France, 2019-10-24 - 2019-10-24. (LA-UR-19-30853)

Schreiber, K. A. Phase Transitions near Absolute Zero: From the Quantum Hall Effect to Gamma Ray Detectors in the Dilution Refrigerator. Presented at *Purdue University Department of Physics Colloquium - Raman Prize for Graduate Students*, Online, Indiana, United States, 2021-04-22 - 2021-04-22. (LA-UR-21-23619)

Posters

Carpenter, M. H., K. E. Koehler, C. J. Fontes, D. G. McNeel, K. A. Schreiber, C. M. Smith, G. L. Wagner, B. Stein, E. G. Bowes, P. Yang, E. R. Batista, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. S. Swetz, D. R. Schmidt, D. T. Becker, J. A. B. Mates, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels, J. Webber and M. P. Croce. Hyperspectral X-ray Imaging: Next-Generation TES Microcalorimeters on the SEM. Presented at *Low-Temperature Detectors 19*, Virtual, New Mexico, United States, 2021-07-19 - 2021-07-30. (LA-UR-21-26481)

Carpenter, M. H., K. G. McIntosh, J. N. Ullom, D. A. Bennett, D. S. Swetz, C. D. Reintsema, J. D. Gard, D. T. Becker, J. A. B. Mates, K. M. Morgan, J. Imrek, A. L. Wessels and M. P. Croce. Development of a Wide-Range X-ray Emission Spectroscopy Measurement System with Transition Edge Sensors and Microwave Multiplexed Readout. Presented at *Low Temperature Detectors 18*, Milan, Italy, 2019-07-22 - 2019-07-26. (LA-UR-19-26750)

Carpenter, M. H., K. G. McIntosh, K. E. Koehler, C. J. Fontes, C. M. Smith, G. L. Wagner, Z. K. Baker, M. L. Handley, M. W. Rabin, M. P. Wilkerson, M. D. Yoho, P. Yang, E. R. Batista, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. S. Swetz, D. R. Schmidt, D. T. Becker, J. A. B. Mates, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels and M. P. Croce. Hyperspectral X-ray Imaging: First

Results and Future Development. Presented at *Applied Superconductivity Conference (ASC) 2020*, Virtual, New Mexico, United States, 2020-10-25 - 2020-11-06. (LA-UR-20-28160)

Croce, M. P., Z. K. Baker, E. R. Batista, M. P. Caffrey, M. H. Carpenter, C. J. Fontes, K. E. Koehler, S. E. Kossmann, S. A. Kozimor, K. G. McIntosh, M. W. Rabin, B. W. Renck, G. L. Wagner, P. Yang, M. D. Yoho, M. P. Wilkerson, D. T. Becker, D. A. Bennett, J. D. Gard, J. Imrek, J. A. B. Mates, K. M. Morgan, G. C. O'Neil, C. D. Reintsema, D. R. Schmidt, D. S. Swetz, A. L. Wessels, J. N. Ullom, R. H. Cantor, J. A. Hall and D. T. Carver. Hyperspectral X-ray Imaging. Presented at *18th International Workshop on Low Temperature Detectors*, Milan, Italy, 2019-07-22 - 2019-07-22. (LA-UR-19-26600)

Koehler, K. E., C. J. Fontes, E. R. Batista, M. H. Carpenter, S. A. Kozimor, K. G. McIntosh, C. M. Smith, G. L. Wagner, P. Yang and M. P. Croce. Dirac-Fock-Slater Calculations for Low Intensity X-ray Features. Presented at *International Workshop on Theory Frontiers in Actinide Sciences*, Santa Fe, New Mexico, United States, 2020-02-02 - 2020-02-05. (LA-UR-20-20828)

McNeel, D. G., M. H. Carpenter, B. Stein, K. E. Koehler, C. J. Fontes, C. M. Smith, G. L. Wagner, M. L. Handley, M. W. Rabin, P. Yang, E. R. Batista, K. A. Schreiber, E. G. Bowes, M. P. Croce, J. N. Ullom, G. C. O'Neil, C. D. Reintsema, D. A. Bennett, G. C. Hilton, D. Swetz, D. R. Schmidt, J. A. B. Mates, D. T. Becker, J. C. Weber, J. D. Gard, K. M. Morgan, J. Imrek, D. Yan, A. L. Wessels and Z. K. Baker. Progress toward absolute calibration of x-ray TESs. Presented at *19th International Workshop on Low Temperature Detectors*, Online, New Mexico, United States, 2021-07-19 - 2021-07-29. (LA-UR-21-26488)

Other

Carpenter, M. H. and M. P. Croce. HXI X1 Data as of November 2019. Dataset. (LA-UR-19-31890)

Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter (U)

Manvendra Dubey
20200035DR

Project Description

The growing threat of a limited nuclear exchange demands 21st century science-tools to assess collateral damage from radioactive fallout that is lethal to humans and potential nuclear winter that could threaten habitability. Nuclear winter is the long-term solar shading, cooling, and drying simulated by global models that prescribe a high-altitude injection of soot form urban fires ignited by the exchange, and is very uncertain. It results from a large fraction of the dark smoke being self-lofted into the stratosphere by solar heating where it can persist for years. In contrast, if the smoke is injected at lower altitudes it rains out rapidly with no nuclear winter. However, in this case the smoke that is mixed with radioactive debris is transported to the surface over long range posing a health hazard. Our goal is to realistically treat the mixing, injection, fate, and transport of mixed smoke-dust produced by low yield exchange for robust assessments. Laboratory measurements of the chemical, optical and microphysical properties of dust-smoke particles using state-of-the-art instruments will be incorporated into our multi-phenomenology fireball, neutron activation, fire, and global atmospheric models. Finally, validation simulations for available observations on 2017 Pacific Northwest megafires and Hiroshima black-rain will be performed.

Publications

Journal Articles

Carrico, C., T. Capek, K. J. Gorkowski, J. T. Lam, S. Gulick, J. M. Karacaoglu, J. E. Lee, C. Dungan, A. C. Aiken, T. Onasch, A. Freedman, C. Mazzoleni and M. K. Dubey. Humidified Single Scattering Albedometer (H-CAPSPMSSA): Design, Data-Analysis, and Validation. Submitted to *Aerosol Science and Technology*. (LA-UR-21-20615)

Chylek, P., C. Folland, J. Klett, G. Lesins and M. K. Dubey. Volcanic eruptions, climate models, and climate geoengineering. Submitted to *Geophysical Research Letters*. (LA-UR-20-24163)

*Chylek, P., C. Folland, M. K. Dubey and J. D. Klett. CMIP5 Climate Models Overestimate Cooling by Volcanic Aerosols. 2020. *Geophysical Research Letters*. **47** (3): e2020GL087047. (LA-UR-19-32146 DOI: 10.1029/2020GL087047)

D'Angelo, G., S. Guimond, J. M. Reisner, D. A. Peterson and M. K. Dubey. Contrasting Stratospheric Smoke Mass and Lifetime from 2017 Canadian and 2019/2020 Australian Megafires: Global Simulations and Satellite Observations. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-21-31453)

Gorkowski, K. J., C. Carrico and M. K. Dubey. Novel Molecular Framework Predicts Organic Aerosol Light Absorption. Submitted to *Nature Communications*. (LA-UR-21-32053)

Huber, R. C., A. C. Aiken, D. M. Dattelbaum, M. K. Dubey, K. J. Gorkowski and D. Podlesak. Particulate Formation During High Explosive Detonations: How Oxygen Balance Drives Parameters Pertinent to Atmospheric Lofting. Submitted to *Scientific Reports*. (LA-UR-21-29162)

*Josephson, A. J., D. Castano, E. Koo and R. R. Linn. Zonal-Based Emission Source Term Model for Predicting Particulate Emission Factors in Wildfire Simulations. 2020. *Fire Technology*. (LA-UR-19-27624 DOI: 10.1007/s10694-020-01024-7)

*Lee, J. E., M. K. Dubey, A. C. Aiken, P. Chylek and C. M. Carrico. Optical and Chemical Analysis of Absorption Enhancement by Mixed Carbonaceous Aerosols in the 2019 Woodbury, AZ, Fire Plume. 2020. *Journal of Geophysical Research: Atmospheres*. **125** (15): e2020JD032399. (LA-UR-20-20021 DOI: 10.1029/2020JD032399)

Lee, J. E., M. K. Dubey, K. J. Gorkowski, K. B. Benedict, A. G. Meyer and A. C. Aiken. Smoke from US wildfires demonstrates significant and predictable light absorption enhancements.. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-22-20288)

McClanahan, T. C., J. T. Goorley and J. D. I. Auxier. Hiroshima and Nagasaki Verification of an Unstructured Mesh based Transmutation Toolkit. Submitted to *Nuclear Technology*. (LA-UR-19-31806)

McClanahan, T. C., J. T. Goorley and J. D. I. Auxier. Comparison of Isotopic Ratios in an Urban Post-Detonation Environment. Submitted to *Journal of Radiation Effects Research and Engineering*. (LA-CP-20-20283)

Reisner, J. M., A. J. Josephson, K. J. Gorkowski, E. Koo, D. Thompson, D. Schroeder and M. K. Dubey. Informed Multi-Scale Approach Applied to the British Columbia Fires of Late Summer 2017. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-22-20272)

*Reisner, J., E. Koo, E. Hunke and M. Dubey. Reply to Comment by Robock et al. on "Climate Impact of a Regional Nuclear Weapon Exchange: An Improved Assessment Based on Detailed Source Calculations". 2019. *Journal of Geophysical Research: Atmospheres*. **124** (23): 12959-12962. (LA-UR-19-26224 DOI: 10.1029/2019JD031281)

Romero, B., S. V. Poroseva, P. Vorobieff and J. M. Reisner. Simulations of the shock-driven Kelvin–Helmholtz instability in inclined gas curtains. Submitted to *Physics of Fluids*. (LA-UR-21-25368)

Conference Papers

McClanahan, T. C. Study of the Production of Radionuclides in Polluted Air from an Urban Nuclear Detonation. Presented at *RPSD 2020*. (Seattle, Washington, United States, 2020-09-13 - 2020-09-17). (LA-UR-20-22003)

Yokelson, D. M., N. Tkachenko, R. W. Robey, Y. W. Li and P. Dub. Performance Analysis of CP2K Code for Ab Initio Molecular Dynamics. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (Supercomputing)*. (St. Louis, Missouri, United States, 2021-11-14 - 2021-11-14). (LA-UR-21-28744)

Reports

Benedict, K. B., M. U. Moosmuller, K. J. Gorkowski and M. K. Dubey. Improved temperature control for measuring the humidity dependence of aerosol optical properties. Unpublished report. (LA-UR-21-28089)

Dubey, M. K., J. J. Benedict, D. O'Malley, B. T. Nadiga, P. A. Johnson, H. S. Viswanathan, P. Chylek and S. Carns. AI for Extreme Volcanic Climate Forcing and Feedback Forecasting in the 21st century. Unpublished report. (LA-UR-21-21384)

Dunning, D. J. Parallelization and Performance Portability in Hydrodynamics Codes. Unpublished report. (LA-UR-20-27394)

Elliott, S. M., C. S. Plesko, T. M. Holland, M. K. Dubey, J. M. Reisner, J. H. Cooley, A. C. Aiken, G. D'Angelo, W. P. Even, C. L. Fryer, G. R. Gisler, K. J. Gorkowski, R. C. Huber, A. J. Josephson, C. M. Mauney, T. C. McClanahan, R. A. Messerly, E. Rougier and E. M. Whitney. Chemistry of Pulses to the Earth Surface Environment: Overview for Next Generation Simulation. Unpublished report. (LA-UR-20-26027)

Gorkowski, K. J., S. H. Jordan, K. B. Benedict and M. K. Dubey. A novel approach to characterize the full spectrum and radiative properties of aerosols. Unpublished report. (LA-UR-21-28132)

McClanahan, T. C. Study of the Production of Isotopes in an Urban Nuclear Post-Detonation Environment. Unpublished report. (LA-UR-20-21439)

Perez, D. M. The Development of a Lagrangian Cloud Physics Package in HiGrad for the Simulation of Pyrocumulonimbus (PyroCb) Cloud. Unpublished report. (LA-UR-21-23587)

Presentation Slides

Aiken, A. C., R. C. Huber, A. M. Schmalzer, M. A. Boggs, J. E. Lee, K. J. Gorkowski and M. K. Dubey. Submicron Soot Microphysical and Chemical Signatures from Detonations of High Explosive Composites. Presented at *38th Annual American Association for Aerosol Research Conference - Virtual Meeting*, Los Alamos, New Mexico, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-27497)

Aiken, A. C., R. C. Huber and J. E. Lee. Physical, optical and chemical signatures of high T and P regime soot for atmospheric detection of high explosive detonations. . (LA-UR-22-20257)

Benedict, K. B. Investigations of Atmospheric Chemistry: Connecting the sources of emissions to impacts.. . (LA-UR-21-31221)

Benedict, K. B., J. E. Lee, K. J. Gorkowski, M. K. Dubey and A. C. Aiken. Emissions from Fires at the Wildland Urban Interface: Laboratory Measurement of Formaldehyde and Aerosol Properties emitted from Building Materials. Presented at *AWMA Atmospheric Optics: Aerosols, Visibility, and the Radiative Balance*, Bryce Canyon, Utah, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-29625)

Benedict, K. B., J. E. Lee, K. J. Gorkowski, M. K. Dubey and A. C. Aiken. Toxic Emissions from Fires at the Wildland Urban Interface: Laboratory Measurement of Formaldehyde and Aerosol from Building Materials. Presented at *American Association for Aerosol Research 2021*, Albuquerque, New Mexico, United States, 2021-10-18 - 2021-10-18. (LA-UR-21-29965)

Benedict, K. B., K. J. Gorkowski, E. Koo, J. M. Reisner, I. J. Simpson, B. Barletta, D. Blake, J. Katich and J. Schwarz. Evidence of secondary organic aerosol formation by non-methane hydrocarbons condensation in Pyro-Cumulonimbus (pyroCb). Presented at *2021 ARM/ASR PI Meeting (online)*, Los Alamos, New Mexico, United States, 2021-06-21 - 2021-06-24. (LA-UR-21-25763)

Benedict, K. B., K. J. Gorkowski, J. E. Lee, I. J. Simpson, B. Barletta, D. R. Blake, G. S. Diskin, J. M. Katich, J. P. Schwartz, J. M. Reisner and M. K. Dubey. Evidence of secondary organic aerosols formation by non-methane hydrocarbons condensation in cold Pyro-Cumulonimbus (pyroCb) outflows. Presented at *EGU 2021*, Vienna, Austria, 2021-04-26 - 2021-04-30. (LA-UR-21-23907)

Benedict, K. B., K. J. Gorkowski, J. E. Lee and M. K. Dubey. Aerosol Properties from Urban Fuels: Experiments at the Solar Furnace and in the CAFE Lab. . (LA-UR-22-20283)

Benedict, K. B., M. U. Moosmuller, K. J. Gorkowski and M. K. Dubey. Improved Temperature Control for Measuring the Humidity Dependence of Aerosol Optical Properties. . (LA-UR-21-27425)

Brown, A. L., H. Mendoza, E. Koo and J. M. Reisner. A High Flux Forest Fire Scenario for Assessing Relative Model Accuracy for CFD Tools. Presented at *Western States Section Combustion Institute (WSSCI)*, Albuquerque, New Mexico, United States, 2019-10-14 - 2019-10-15. (LA-UR-19-30060)

Dubey, M. K. Field Observations of Climate Forcing by Fires, Forests, Fossil Energy & Food Production. Presented at *Texas A&M University Atmospheric Science Seminar*, College Station, Texas, United States, 2020-01-29 - 2020-01-29. (LA-UR-20-20735)

Dubey, M. K. Nuclear Winter and Geoengineering Climate: Lessons from Volcanoes and Megafires. Presented at *LANL Fellows Meeting*, Los Alamos, New Mexico, United States, 2021-07-20 - 2021-07-20. (LA-UR-21-27043)

Dubey, M. K., A. C. Aiken, K. J. Gorkowski, J. E. Lee, T. Capek and C. Carrico. TRacking Aerosol Convection interactions ExpeRiment (TRACER): Carbon Aerosol Thrust (CAT). Presented at *ARM TRACER WORKSHOP (Virtual)*, Los Alamos, New Mexico, United States, 2020-04-20 - 2020-04-21. (LA-UR-20-22994)

Dubey, M. K., G. D'Angelo, S. Guimond, K. J. Gorkowski, J. M. Reisner and D. Peterson. Stratospheric Smoke Mass, Lifetime & Cooling from 2017 British Columbia & 2019 New South Wales Megafires: Global Simulations & Satellite Observations. Presented at *American Meteorological Society Annual Meeting*, Houston, Texas, United States, 2022-01-24 - 2022-01-28. (LA-UR-22-20622)

Dubey, M. K., G. D'Angelo, S. R. Guimond, D. Peterson and J. M. Reisner. Stratospheric Smoke Injection above British Columbia and Australia: Mechanisms and Impacts. Presented at *American Geophysical Union (AGU) Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32131)

Dubey, M. K., J. J. Benedict, D. O'Malley, B. T. Nadiga, P. A. Johnson, H. S. Viswanathan and S. Carns. AI for Extreme Volcanic Climate Forcing & Feedback Forecasts in the 21st century. Presented at *AI4ESP Workshop DOE Office of Science*, Washington, District Of Columbia, United States, 2021-11-09 - 2021-11-15. (LA-UR-21-30758)

Dubey, M. K., J. M. Reisner, E. Koo, S. Guimond, A. C. Aiken, G. D'Angelo, D. Peterson and M. Fromm. Transport, Composition and Lifetime of Extreme Wildfire Smoke to Assess their Impacts. Presented at *AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32202)

Dubey, M. K., K. J. Gorkowski, J. M. Reisner, K. B. Benedict, A. J. Josephson, E. Koo, G. D'Angelo, D. Peterson and S. R. Guimond. Condensation in Pyro-cumulonimbus Outflow Explains Large Stratospheric Smoke Mass Injection and Thickly Coated Black Carbon. Presented at *EGU annual meeting*, Vienna, Austria, 2021-04-25 - 2021-04-30. (LA-UR-21-23940)

Dubey, M. K., K. J. Gorkowski, J. M. Reisner, K. B. Benedict, A. J. Josephson and E. Koo. Large SOA Formation by Vapor Condensation in PyroCb outflow in LES Simulations and in situ Airborne Data. Presented at *ASR ARM Science Team Meeting*, Germantown, Maryland, United States, 2021-06-21 - 2021-06-24. (LA-UR-21-25802)

Dubey, M. K., K. J. Gorkowski and S. Guerin. Looking Within the Medio Fire Smoke Plume at Los Alamos National Laboratory. . (LA-UR-20-26772)

Dubey, M. K. and J. M. Reisner. Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter. Presented at *LDRD-DR 1st year progress review*, Los Alamos, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20046)

Dubey, M. K. and J. M. Reisner. (U) Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter (20200035DR) 3rd Year Review. . (LA-UR-22-20329)

Gonzales, R. L. HIGRAD: High Gradient Flow Solver, Poisson FFT Solver. . (LA-UR-21-27745)

Gorkowski, K. J., K. B. Benedict, J. E. Lee, A. C. Aiken, C. Carrico, T. Capek and M. K. Dubey. Humidity-Dependent Brown Carbon Light Absorption and Photobleaching: Laboratory and Model Synthesis of Organic Dyes.. Presented at *American Association for Aerosol Research 39th annual conference*, Albuquerque, New Mexico, United States, 2021-10-18 - 2021-10-22. (LA-UR-21-29966)

Gorkowski, K. J., K. B. Benedict, J. E. Lee, A. C. Aiken, C. Carrico and M. K. Dubey. Laboratory and Model Synthesis of Brown Carbon Dyes: Humidity-Dependence and Photobleaching. Presented at *Air and Waste Management Association: Atmospheric Optics: Aerosols, Visibility, and the Radiative Balance*, Bryce Canyon, Utah, United States, 2021-10-04 - 2021-10-08. (LA-UR-21-29546)

Gorkowski, K. J., K. B. Benedict, S. H. Jordan and M. K. Dubey. Vertical profiles of soot reveal complex aerosol microphysics. Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2022-01-18 - 2022-01-18. (LA-UR-22-20316)

Gorkowski, K. J., M. K. Dubey, T. Capek, C. Carrico, K. B. Benedict, J. E. Lee and A. C. Aiken. Observing RH-Dependent Absorbing Aerosol Optics: Gray and Brown Carbon, and TRACER-CAT. Presented at *2021 ARM/ASR PI Meeting*, online, New Mexico, United States, 2021-06-21 - 2021-06-24. (LA-UR-21-25281)

Josephson, A. J., E. Koo, D. K. Thompson and J. M. Reisner. Aerosol Formation and Ejection via Pyrocumulonimbus Clouds in the British Columbia Fires of Late Summer 2017. Presented at *AAAR 38th Annual Conference*, Los Alamos, New Mexico, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-28540)

Josephson, A. J., J. M. Reisner, E. Koo and K. J. Gorkowski. Multi-Scale Simulations of Aerosol Lofting & Production by 2017

British Columbia PyroCbs Match Observations of aerosol lofting and production (and BC21 PyroCb) Modeling and Simulations - Informed Hiroshima Fallout Simulations. . (LA-UR-22-20287)

Josephson, A. J. and R. R. Linn. Modeling Soot Emissions in Coarse Grid Simulations. Presented at *2019 Fall Technical Meeting of the Western States Section of the Combustions Institute*, Albuquerque, New Mexico, United States, 2019-10-14 - 2019-10-15. (LA-UR-19-30398)

Koo, E. LDRD-DR Project: Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter. Presented at *Invited Talk to Mechanical Engineering Dept, University of New Mexico.*, Albuquerque, New Mexico, United States, 2021-01-29 - 2021-01-29. (LA-UR-21-20956)

Koo, E. CY2020 Institutional Computing Annual Progress Report: Multi-scale turbulent atmospheric interactions (w19_atmo_turbulence, renewed as w21_atmoturb). . (LA-UR-21-21906)

Koo, E. British Columbia 2021 Fire Pyrocumulonimbus HIGRAD Simulation - Visualization. . (LA-UR-21-31598)

Koo, E., R. W. Robey and A. J. Josephson. Computational Advances for High-Fidelity Simulations. Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2022-01-18 - 2022-01-18. (LA-UR-22-20303)

Lee, J. E., M. K. Dubey, K. J. Gorkowski, K. B. Benedict and A. C. Aiken. Smoke from US wildfires demonstrates significant and predictable light absorption enhancements. . (LA-UR-22-20240)

Linn, R. R. and M. K. Dubey. Fire Predictions and Impacts. . (LA-UR-21-30176)

McClanahan, T. C. Study of the Production of Isotopes in an Urban Nuclear Post- Detonation Environment. . (LA-UR-20-22421)

McClanahan, T. C., J. M. Reisner, E. Koo and M. K. Dubey. Path Forward: Hiroshima Nuclear Activation, Exposure, Black Rain Fallout Simulations and Chemical Analysis. Presented at *LDRD DR Mid year Appraisal*, Los Alamos, New Mexico, United States, 2021-01-07 - 2021-01-07. (LA-UR-21-20076)

Perez, D. M. Cloud Microphysics Considerations for Simulating Pyrocumulonimbus Clouds in HIGRAD. . (LA-UR-20-27338)

Perez, D. M. The Development of a Lagrangian Cloud Microphysics Package in HiGrad for the Simulation of PyroCumulonimbus (PyroCb) Clouds. . (LA-UR-21-29743)

Reisner, J. M. Towards Modeling Complex Fallout: Model Description and Preliminary Results. Presented at *JOWOG 43*, Los Alamos, New Mexico, United States, 2020-01-06 - 2020-01-06. (LA-CP-20-20000)

Reisner, J. M. Nuclear Winter Update: Post Reisner et al. (2018) JGR paper. . (LA-UR-20-23077)

Reisner, J. M. Megafires: A New Fire Paradigm. . (LA-UR-21-31339)

Yokelson, D. M. CP2K Performance Optimization. Presented at *Parallel Computing Student Project Outbrief*, Los Alamos, New Mexico, United States, 2021-08-05 - 2021-08-05. (LA-UR-21-27535)

Posters

Aiken, A. C., M. K. Dubey, J. E. Lee, R. C. Huber and T. L. Williamson. Detonation Soot Chemistry using High Time-Resolution Aerosol Mass Spectrometry. Presented at *Carbon in Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-10-28 - 2019-10-28. (LA-UR-19-31002)

Aiken, A. C., R. C. Huber, A. M. Schmalzer, M. A. Boggs, J. E. Lee, K. J. Gorkowski and M. K. Dubey. High Temperature and Pressure Regime Soot Microphysical and Chemical Analysis for Real-Time Atmospheric Detection of High Explosives. Presented at *AGU Fall Meeting*, los alamos, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29713)

Dubey, M. K., P. Chylek, G. D'Angelo, S. R. Guimond and J. M. Reisner. Evaluating Aerosol Solar Reflection Climate Models by Post Stratospheric Mass Injection Response Observations. Presented at *AGU Fall Meeting*, Washington, District Of Columbia, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29624)

Lee, J. E., M. K. Dubey, A. C. Aiken, K. J. Gorkowski and C. Carrico. Black carbon aerosol mixing state in fresh and aged wildfire smoke: Harmonizing Instruments, Laboratory and Field Studies. Presented at *AGU 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-18. (LA-UR-20-29833)

Lee, J. E., M. K. Dubey, K. J. Gorkowski, K. B. Benedict and A. C. Aiken. Smoke from Western US wildfires demonstrates significant and predictable light absorption enhancements. Presented at *AGU 2021*, online, New Mexico, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32247)

Perez, D. M., E. Koo, J. M. Reisner and J. M. Canfield. The Development of a Lagrangian Cloud Physics Package in LANL's High Gradient (HiGrad) Model for Wildfire Simulations. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31997)

Other

Lee, J. E., M. K. Dubey and A. C. Aiken. Datafiles for: Optical and chemical analysis of absorption enhancement by mixed carbonaceous aerosols in the 2019 Woodbury, AZ fire plume. Dataset. (LA-UR-20-20454)

Capturing the Origin and Evolution of Persistence Using Real-time, In vivo, Single Cell Transcriptomics

Murray Wolinsky
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Project Description

Antimicrobial and anticancer therapies frequently fail due to tiny numbers of cells which persist despite treatment. Current analysis (transcriptomic) methods are blind to the existence and behavior of these crucial actors ("persisters") unless infeasible numbers of cells are employed. Improving therapies requires developing new methods. Our effort will identify and study the persisters that determine the fate of populations using novel technology developed for that purpose. Existing methods of transcriptomics are inadequate. But a radically new approach has only recently become possible: the ability to monitor the internal state of individual cells and to do this for many cells in real time. We will mature this latent technology, drawing on critical Los Alamos innovations. Our project is organized to perform foundational studies using our transformational new approach. We will observe the temporal dynamics of gene expression in single cells in vivo. Our method is called RIVOT (Real-time In VivO Transcriptomics). We will identify each gene expression event of interest by generating bar-coded signals as it occurs. We will watch expression of multiple (~10) targeted genes simultaneously. Our effort will not only provide unprecedented insight into persistence, it will revolutionize the study of gene expression in doing so.

Publications

Journal Articles

Kalb, D. M., H. Vo, S. H. Adikari, E. Hong-Geller, B. munsky and J. H. Werner. Visualization and Modeling of Inhibition of IL-1\xce\xb2 and TNF\xce\xb1 mRNA Transcription at the Single-Cell Level. Submitted to *Scientific Reports*. (LA-UR-20-28135)

Morales, D. P., S. H. Adikari, J. H. Werner, M. A. Wolinsky, I. Ojima, J. Kim, E. Hong-Geller and S. N. Micheva-Viteva. Targeting bet-hedging in Burkholderia spp with taxane-based inhibitors of efflux activity enhances antibiotic efficiency and ameliorates bacterial persistence in vitro.

Submitted to *Antimicrobial Agents and Chemotherapy*. (LA-UR-22-20696)

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

Conference Papers

Strauss, C. E. and J. Morton. Protein Structural Alignments From Sequence. Presented at *NeuroIPS: Thirty-fourth Conference on Neural Information Processing Systems*. (Virtual, New Mexico, United States, 2020-12-06 - 2020-12-12). (LA-UR-20-28603)

Presentation Slides

Banerjee, S. and R. K. Jha. Transporter Modeling and Design For Designer Cargo. Presented at *Visualizing Living Systems*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21867)

Bolding, M. R. Persistence in Cancer. Presented at *Workshop on Visualizing Living Systems*, Virtual, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21823)

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

Hennelly, S. P. Engineering a Semi-synthetic Organism for Real-time detection of Gene expression.. Presented at *Visualizing Living Systems Workshop*, LOS ALAMOS, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21711)

Hennelly, S. P. Engineering a Semi-synthetic Organism for Real-time detection of Gene expression.. Presented at *Worksop on Visualizing Living Systems*, LOS ALAMOS, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22011)

Kumar, A., S. P. Hennelly and N. A. Pace. Integration and Maintenance of unnatural base pairs (UBPS) Inside the Living Cell. Presented at *Workshop on Visualizing Living*

Systems draft agenda, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22580)

Morales, D. P., S. N. Micheva-Viteva, M. A. Wolinsky and J. H. Werner. Measuring gene expression involved in bacterial persistence at the single cell level. Presented at *Visualizing Living Systems Workshop*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-21719)

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

Werner, J. H. Methods to Visualize 3D Dynamics. Presented at *Northern Arizona University Seminar*, Virtual, New Mexico, United States, 2020-10-22 - 2020-10-22. (LA-UR-20-28259)

Wolinsky, M. A. welcome and Introduction to the LANL Workshop on Visualizing Living Systems. Presented at *LANL Workshop on Visualizing Living Systems*, Los Alamos, New Mexico, United States, 2021-02-25 - 2021-02-25. (LA-UR-21-22713)

Posters

Micheva-Viteva, S. N. and E. Hong-Geller. In Pursuit of Effective Host-Directed Therapies Against Human Pathogens. Presented at *CBD&T Conference*, Cincinati, Ohio, United States, 2019-11-18 - 2019-11-22. (LA-UR-19-31135)

The Mini Astrophysical Mega Electron-volt Background Observatory (MAMBO) CubeSat Mission: Demonstrating Agile Satellite Platforms for Astrophysics and National Security

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Project Description

Gamma-ray sensing from space is a critical capability for the Nation's national security and scientific missions. Though vital for both the detection of exo-atmospheric nuclear detonations and the study of energetic astrophysical phenomena, high-quality gamma-ray measurements in space are technically challenging due to the intense radiation fields that exist above the atmosphere. The entire spacecraft is bombarded by high-energy particles from deep space and the Sun, causing it to glow so brightly in gamma-rays that weak signals of interest are often obscured. The Mini Astrophysical MeV Background Observatory (MAMBO) mission will demonstrate a new approach to detecting gamma rays in space by flying an innovative detector on a "CubeSat," a satellite no bigger than a microwave oven and weighing less than 50 pounds. Such a small spacecraft will glow much less brightly. We will validate this approach via a challenging astronomical observation: the best-ever measurement of the mysterious, faint gamma-ray "background" emanating from the distant Universe. MAMBO will thus provide an important scientific result while demonstrating a new, flexible paradigm for space-based sensing for national security missions such as the National Nuclear Security Administration's space-based nuclear detonation detection (SNDD) program.

Publications

Journal Articles

Bloser, P. F., W. Thomas Vestrand, M. P. Hehlen, L. P. Parker and A. S. Hoover. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat mission. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-29829 DOI: 10.1117/12.2576143)

Conference Papers

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker, D. T. Beckman, J. M. McGlown, L. Holguin, K. K. Katko, J. D. Sedillo, A. E. Nelson and G. K. Lee. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *35th Annual Small Satellite Conference*. (Online, New Mexico, United States, 2021-08-07 - 2021-08-12). (LA-UR-21-25162)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker, D. T. Beckman, J. M. McGlown, L. Holguin, K. K. Katko, J. D. Sedillo, A. E. Nelson and G. K. Lee. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat mission. Presented at *SPIE Optics + Photonics: UV, X-Ray, and Gamma-Ray Space Instrumentation for Astronomy XXII*. (San Diego, California, United States, 2021-08-01 - 2021-08-06). (LA-UR-21-26690)

Reports

Fryer, C. L. MAMBO Institutional Computing Progress Report. Unpublished report. (LA-UR-22-20974)

Hehlen, M. P. and K. K. Katko. Formal Request for Information (RFI): Ground Stations for LANL CubeSats. Unpublished report. (LA-UR-21-26278)

Presentation Slides

Bloser, P. F. Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission (. Presented at *35th Annual Small Satellite Conference*, Online, New Mexico, United States, 2021-08-07 - 2021-08-12. (LA-UR-21-25964)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker, D. T. Beckman, J. D. Sedillo, J. M. McGlown, L. Holguin, J. M. Michel, A. E. Nelson and D. C. Poulson. Let's MAMBO (Mini Astrophysical MeV Background Observatory)! A New CubeSat Mission at Los Alamos National Laboratory. Presented at *The 37th Annual New Mexico Symposium*, Online, New Mexico, United States, 2021-11-19 - 2021-11-19. (LA-UR-21-31383)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker and A. S. Hoover. The Mini Astrophysical MeV Background Observatory (MAMBO) CubeSat Mission. Presented at *2020 IEEE Nuclear Science Symposium (NSS) and Medical Imaging Conference (MIC)*, Online, New Mexico, United States, 2020-10-31 - 2020-11-07. (LA-UR-20-28737)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker and
A. S. Hoover. The Mini Astrophysical MeV Background
Observatory (MAMBO) CubeSat Mission. Presented at *The
36th Annual New Mexico Symposium*, Online, New Mexico,
United States, 2020-11-13 - 2020-11-13. (LA-UR-20-29224)

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, L. P. Parker and
A. S. Hoover. The Mini Astrophysical MeV Background
Observatory (MAMBO) CubeSat Mission. Presented at
SPIE Astronomical Telescopes + Instrumentation, Online,
New Mexico, United States, 2020-12-13 - 2020-12-18. (LA-
UR-20-29730)

Posters

Bloser, P. F., W. T. Vestrand, M. P. Hehlen, K. K. Katko, L. P. Parker,
D. T. Beckman, J. D. Sedillo, J. M. McGlown, J. M. Michel,
R. H. Scobie, A. E. Nelson, D. C. Poulson, T. J. Roth, C. L.
Fryer, A. L. Hungerford and M. R. Mumpower. The Mini
Astrophysical MeV Background Observatory (MAMBO)
CubeSat Mission. Presented at *19th Divisional Meeting
of the High Energy Astrophysics Division*, Pittsburgh,
Pennsylvania, United States, 2022-03-13 - 2022-03-17. (LA-
UR-22-22176)

HEROS - Human Exposure of Radiation using Organ Systems

Jennifer Harris
20210204DR

Project Description

We will develop an integrated system for biosignature discovery, comprehensive assessment, empirical measurement and evaluation of radiation exposure on human beings by combining three novel technology portfolios: organs on a chip, theoretical modeling and empirical rad-bio measurements. Individual milestone scientific innovations include: 1) development of a first-of-its-kind integrated modeling system to compute organ-specific radiological dose in urban environments, accounting for complexity of the environment; 2) discovery of biosignatures of radiation exposure, as a function of time and dose for rapid assessment of human health impacts in a reliable manner; and 3) validation of human organ models as a physiologically relevant substitute to animal studies. Our project can resolve some of the big challenges in this field. Bioengineered organs will create a first ever capability to study radiation biology directly in human tissue. The suites of biomarkers identified could transform early exposure identification, and countermeasure development. Integration of modeling with experimentation will result in a unique human radiological dose capability for assessments across unprecedented scales. Thus, this project can integrate scientific innovation to actionable response and has the potential to initiate new research efforts in hazard response, training exercises for radiological disasters, and assessments for medical and decontamination communities.

Publications

Journal Articles

Brambilla, S., M. A. Nelson, P. T. Conry, N. Duboc and M. J. Brown. Dirty bomb source term characterization and downwind dispersion: review of experimental evidence. Submitted to *Journal of Environmental Radioactivity*. (LA-UR-21-31129)

Presentation Slides

Akhadov, L. E. Summary of Research Experience. . (LA-UR-21-30606)

Brambilla, S. and M. J. Brown. Relevance of Laboratory Data for Estimating Particle Resuspension from Outdoor Surfaces. Presented at *24th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling*, Fairfax, Virginia, United States, 2020-12-08 - 2020-12-10. (LA-UR-20-30022)

Coombs, K. E. Microphysiological Systems and Mechanobiology. . (LA-UR-21-23309)

Posters

Moore, S. C., L. M. Lilley, H. Mukundan and J. F. Harris. Chemical or Radiological Toxicity: Effects of Uranium Oxides on Human Lung Cells. Presented at *American Chemical Society (ACS) National Meeting & Exposition - Spring*, San Diego, California, United States, 2022-03-20 - 2022-03-20. (LA-UR-22-22533)

Basic Science of Underground Nuclear Explosions: Emplacement Condition Signature Discovery

Thomas Rahn
20210215DR

Project Description

The research proposed in this project will support national security and stockpile stewardship by increasing our understanding of the behavior of material surrounding an Underground Nuclear Explosion (UNE). Although many parts of a UNE have been studied, there are key gaps that warrant more research, and one of these will be explored as part of this project. Through both measurement of gaseous inclusions and actinide isotopes in debris plus simulations of up to thousands of isotopes generated during the event producing the debris, a comparative assessment of the results will indicate what areas we still need to study more thoroughly.

Publications

Reports

Rahn, T. A., H. B. D. Miller and D. L. Eldridge. A CRUSHING AND GAS SEPARATION VACUUM LINE SYSTEM FOR THE PURIFICATION AND STUDY OF GASES IN ROCK SAMPLES. Unpublished report. (LA-UR-21-31695)

Presentation Slides

Boukhalfa, H., A. Migdissov and C. E. Campe. Partitioning of Actinides and Metals Between the Vapor Phase and the Melt. . (LA-UR-21-31900)

Tutt, J. R. and T. C. McClanahan. Activation Calculations using MCNP Unstructured Mesh Geometries. Presented at *2021 MCNP\xc2\xae User Symposium (Virtual)*, Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26603)

Posters

Armstrong, J. C., J. R. Tutt and T. C. McClanahan. MCNP Unstructured Mesh Applications and Activation Calculations. Presented at *2021Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25742)

Armstrong, J. C., J. R. Tutt and T. C. McClanahan. MCNP Unstructured Mesh Applications and Activation Calculations. Presented at *2021Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25742)

Armstrong, J. C., J. R. Tutt and T. C. McClanahan. MCNP Unstructured Mesh Applications and Activation Calculations. Presented at *2021Engineering Capability Review*, Los Alamos, New Mexico, United States, 2021-06-29 - 2021-07-01. (LA-UR-21-25742)

Atomtronics: A New Approach to Sensing, Signal Processing, and Signal Analysis

Malcolm Boshier
20180045DR

Project Description

The project addresses three challenges facing the intelligence and defense communities: navigation when global position system (GPS) is unavailable or denied, unscrambling mixtures of radio signals received by multiple antennas (Blind Source Separation, or BSS), and determining the security of cryptography systems that rely on the presumed hardness of finding the prime factors of a large number. Our proposed solutions are based on atomtronics, the emerging science of circuits created from atoms flowing inside guides. We expect to demonstrate a compact atomtronic rotation sensor that outperfroms all existing technologies and therefore improves the accuracy of inertial navigation. We plan to build a prototype atomtronic signal processing circuit that can perform BSS. Finally, we will build an atomtronic device that finds the prime factors of numbers larger than any factored to date on quantum computers.

Technical Outcomes

This project used cold atom technology to advance the state-of-the-art in atomtronics. First, the team demonstrated the world's first waveguide matter wave Sagnac atom interferometer. Second, the team showed that an atom interferometer based on a non-interacting gas can have an interrogation time an order of magnitude longer than previously observed. Third, the team visualized the wavefunction dynamics of a resonantly driven quantum system and demonstrated an unprecedented level of control over it.

Publications

Journal Articles

Boshier, M. G., M. C. Cassidy and L. E. Harrell. Improved optical standing-wave beam splitters for Bose-Einstein condensates. Submitted to *Journal of Applied Physics*. (LA-UR-21-25104)

Kim, H., K. A. Krzyzanowska, C. Ryu, K. C. Henderson, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple-loop atom interferometer. Submitted to *arXiv.org*. (LA-UR-20-28166)

Kim, H., K. A. Krzyzanowska, K. C. Henderson, C. Ryu, E. M. E. Timmermans and M. G. Boshier. One second interrogation time in a 200 round-trip waveguide atom interferometer. Submitted to *Physical Review Letters*. (LA-UR-22-20692)

Krzyzanowska, K. A., J. Ferreras, C. Ryu, C. Samson and M. G. Boshier. Experimental Realization of a BEC Optical Waveguide Sagnac Atom Interferometer. Submitted to *Physical Review A*. (LA-UR-21-28874)

*Ryu, C., E. C. Samson and M. G. Boshier. Quantum interference of currents in an atomtronic SQUID. 2020. *Nature Communications*. **11** (1): 3338. (LA-UR-20-25170 DOI: 10.1038/s41467-020-17185-6)

Presentation Slides

Boshier, M. G. DOE HEP and Quantum Sensing Research at Los Alamos National Laboratory. Presented at *Argonne Workshop on Quantum Sensing*, Chicago, Illinois, United States, 2017-12-12 - 2017-12-12. (LA-UR-17-31155)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31463)

Boshier, M. G. Two Experiments in Atomtronics: Quantum Interference in an Atomtronic SQUID and a Waveguide Sagnac Atom Interferometer. Presented at *2019 Benasque Atomtronics Workshop*, Benasque, Spain, 2019-05-05 - 2019-05-17. (LA-UR-19-24576)

Boshier, M. G. Lessons Learned From Developing Quantum Sensors. Presented at *STEP Workshop on Quantum Sensors*, McLean, Virginia, United States, 2019-09-10 - 2019-09-10. (LA-UR-19-29036)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *Quantum Technologies and Sensing Workshop*, Manchester, United Kingdom, 2019-10-27 - 2019-10-27. (LA-UR-19-30772)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *Seminar at Purdue University*, West Lafayette, Indiana, United States, 2019-11-12 - 2019-11-12. (LA-UR-19-31593)

Boshier, M. G. A Moving Waveguide Sagnac Atom Interferometer. Presented at *Workshop on Inertial Sensing*,

Brighton, United Kingdom, 2019-11-29 - 2019-11-29. (LA-UR-19-32050)

Boshier, M. G., C. Ryu and C. Samson. Quantum \xc2\xa0Interference\xc2\xa0in\xc2\xa0an \xc2\xa0Atomtronic\xc2\xa0SQUID. Presented at *PQE-2018*, Snowbird, Utah, United States, 2018-01-08 - 2018-01-12. (LA-UR-18-20219)

Boshier, M. G. and C. Ryu. Atomtronics for Quantum Sensing. Presented at *2018 CINT User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-29086)

Henderson, K. C. Symmetry and How it Breaks. Presented at *New Mexico History Museum*, Santa Fe, New Mexico, United States, 2019-02-22 - 2019-02-22. (LA-UR-19-21059)

Kim, H. Detailed balance of thermalization dynamics in Rydberg quantum simulators. Presented at *LANL Quantum DAY*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31537)

Kim, H. Waveguide atom interferometer at LANL. . (LA-UR-21-22793)

Krzyzanowska, K. A. Atomtronic circuits with optical dipole potentials. Presented at *Atomtronics@AbuDhabi2021*, AbuDhabi, United Arab Emirates, 2021-05-31 - 2021-06-11. (LA-UR-21-27040)

Kurkcuoglu, D. M. Quantum simulation and quantum technologies with cold atoms. . (LA-UR-20-22384)

Martin, M. J., C. Ryu and M. G. Boshier. Quantum technologies with ultracold atoms. Presented at *UC Quantum Information Science Research Workshop*, Berkeley, California, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24127)

Posters

Boshier, M. G. and C. Ryu. Sensing with Atomtronics Circuits and Devices. Presented at *SOS capability review*, Los Alamos, New Mexico, United States, 2018-04-24 - 2018-04-25. (LA-UR-18-23422)

Cassidy, M. C. Presentation2. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27193)

Hurd, S. J. Optimum Transportation of Cold Atoms. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27140)

Hurd, S. J. symposium poster sara hurd 2019. Presented at *Student Symposium*, Las Alamos, New Mexico, United States, 2019-08-07 - 2019-08-07. (LA-UR-19-27933)

Kim, H., J. Ferreras Fuertes, K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu and M. G. Boshier. Progress Toward Atomtronics Sagnac Interferometer. Presented at *2019 Postdoc Research Symposium and Career Fair*,

Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28645)

Kim, H., K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple round-trip waveguide atom interferometer. Presented at *APS DAMOP 2020*, Portland, Oregon, United States, 2020-06-01 - 2020-06-01. (LA-UR-20-23957)

Kurkcuoglu, D. M. Unconventional color superfluidity in ultra-cold fermions: Quintuplet pairing, quintuple point and pentacriticality. Presented at *39th CNLS Strongly Correlated Systems Conference*, Santa Fe, New Mexico, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-23837)

Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces

Abul Azad
20180062DR

Project Description

Modern communication, sensing, and surveillance systems rely heavily on the utilization of the electromagnetic spectrum for collecting information, controlling instruments, and making decisions. Our proposed spatio-temporal modulated metasurfaces will result in a revolutionary design paradigm that will enable the effective control and manipulation of electromagnetic waves, and hence play a critical role in attaining enhanced performance of electromagnetic systems. In particular, we will apply this technology to small satellite platforms, an emerging geo-spatial capability for remote sensing and imaging which are a key component of Los Alamos National Laboratory mission space in Science of Signatures. However, they are intrinsically constrained in size, weight, and power, and are in dire need of revolutionary design paradigms to enable dramatically increased performance. This project underpins the Laboratory mission in Science supporting National Security, and advances sensing capabilities for space situational awareness in Global Security. The main anticipated outcomes of this research are reprogrammable microwave metasurface antennas for active beam steering and wavefront correction, and control over their transmission and reception characteristics through tailored modulations in space and time.

Technical Outcomes

This project modeled phase-gradient metasurfaces for wavefront control; demonstrated a static metasurface reflectarray for focusing/collimation, a linear-to-circular polarization converter based on a reflective metasurface, and a veri-focal Alvarez lens, a design control system for active and dynamic metasurfaces, and a nonreciprocal metasurface for wavefront control; developed and demonstrated modulation protocols for high-efficiency nonreciprocal conversion of harmonics; prototyped a deployable high-gain antenna for SmallSat platform; and developed theory for nonreciprocal metasurfaces and space-time quantum metasurfaces.

Publications

Journal Articles

Banerjee, S., N. L. Abhishikth, S. Karmakar, D. Kumar, S. Rane, S. Goel, A. K. Azad and D. R. Chowdhury. Modulating Extraordinary Terahertz Transmissions in Multilayer Plasmonic Metasurfaces. Submitted to *Journal of Optics*. (LA-UR-20-27953)

*Cardin, A. E., S. R. Silva, S. R. Vardeny, W. J. Padilla, A. Saxena, A. J. Taylor, W. J. M. Kort-Kamp, H. Chen, D. A. R. Dalvit and A. K. Azad. Surface-wave-assisted nonreciprocity in spatio-temporally modulated metasurfaces. 2020. *Nature Communications*. **11** (1): 1469. (LA-UR-19-30765 DOI: 10.1038/s41467-020-15273-1)

*Chang, C., W. J. M. Kort-Kamp, J. Nogan, T. S. Luk, A. K. Azad, A. J. Taylor, D. A. R. Dalvit, M. Sykora and H. Chen. High-Temperature Refractory Metasurfaces for Solar Thermophotovoltaic Energy Harvesting. 2018. *Nano Letters*. **18** (12): 7665-7673. (LA-UR-18-27846 DOI: 10.1021/acs.nanolett.8b03322)

*Chang, C., Z. Zhao, D. Li, A. J. Taylor, S. Fan and H. Chen. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. 2019. *Physical Review Letters*. **123** (23): 237401. (LA-UR-18-31108 DOI: 10.1103/PhysRevLett.123.237401)

Chen, H., S. R. M. Silva, C. Corbella, A. D. Tang, P. Nath and A. K. Azad. Microwave Metasurface-Based Alvarez Lens. Submitted to *Applied Physics Letters*. (LA-UR-20-30096)

Chen, H., W. J. de Melo Kort-Kamp, D. A. R. Dalvit, A. K. Azad, C. Chang, J. Nogan, Z. Yang, W. Ross and T. S. Luk. Highly Plasmonic Titanium Nitride by Room-Temperature Sputtering. Submitted to *Scientific Reports*. (LA-UR-19-29707)

Chen, H., Z. Zhao, D. Li, A. J. Taylor, S. Fan and C. Chang. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective

Metasurfaces. Submitted to *Physical Review Letters*. (LA-UR-19-29771)

*Chen, X., S. Ghosh, Q. Xu, C. Ouyang, Y. Li, X. Zhang, Z. Tian, J. Gu, L. Liu, A. K. Azad, J. Han and W. Zhang. Active control of polarization-dependent near-field coupling in hybrid metasurfaces. 2018. *Applied Physics Letters*. **113** (6): 061111. (LA-UR-18-29890 DOI: 10.1063/1.5040162)

Cheong, S., D. Talbayev, V. Kiryukhin and A. Saxena. Broken symmetries, non-reciprocity, and multiferroicity. 2018. *npj Quantum Materials*. **3** (1): 19. (LA-UR-18-20267 DOI: 10.1038/s41535-018-0092-5)

R. Dalvit, D. A., F. Intravaia and K. Busch. Fluctuation-induced phenomena in photonic systems: Introduction. Submitted to *Journal of the Optical Society of America B: Optical Physics*. (LA-UR-19-23024)

Dandoloff, R. and A. Saxena. XY Model on Interacting Parallel Planes with a Soliton. Submitted to *Physics Letters. Section A: General, Atomic and Solid State Physics*. (LA-UR-17-31143)

*Belen Farias, M., W. J. M. Kort-Kamp and D. A. R. Dalvit. Quantum friction in two-dimensional topological materials. 2018. *Physical Review B*. **97** (16): 161407. (LA-UR-17-29840 DOI: 10.1103/PhysRevB.97.161407)

*Gaididei, Y., V. P. Kravchuk, F. G. Mertens, O. V. Pylypovskyi, A. Saxena, D. D. Sheka and O. M. Volkov. Localization of magnon modes in a curved magnetic nanowire. 2018. *Low Temperature Physics*. **44** (7): 634-643. (LA-UR-18-20270 DOI: 10.1063/1.5041428)

*Intravaia, F., M. Oelschlaeger, D. Reiche, D. A. R. Dalvit and K. Busch. Quantum Rolling Friction. 2019. *Physical Review Letters*. **123** (12): 120401. (LA-UR-18-29152 DOI: 10.1103/PhysRevLett.123.120401)

*M. Kort-Kamp, W. J., F. J. Culchac, R. B. Capaz and F. A. Pinheiro. Photonic spin Hall effect in bilayer graphene moir\xc3\xa9 superlattices. 2018. *Physical Review B*. **98** (19): 195431. (LA-UR-18-27864 DOI: 10.1103/PhysRevB.98.195431)

de Melo Kort-Kamp, W. J., A. K. Azad and D. A. R. Dalvit. Space-Time Quantum Metasurfaces. Submitted to *Nature Photonics*. (LA-UR-21-20535)

*Ledwith, P., W. J. M. Kort-Kamp and D. A. R. Dalvit. Topological phase transitions and quantum Hall effect in the graphene family. 2018. *Physical Review B*. **97** (16): 165426. (LA-UR-17-30904 DOI: 10.1103/PhysRevB.97.165426)

Muniz, Y., A. Manjavacas, C. Farina, D. A. R. Dalvit and W. J. de Melo Kort-Kamp. Unraveling the decay mechanisms of two-quanta spontaneous photonic transitions. Submitted to *Nature Photonics*. (LA-UR-20-20456)

*Muniz, Y., F. S. S. da Rosa, C. Farina, D. Szilard and W. J. M. Kort-Kamp. Quantum two-photon emission in a photonic cavity. 2019. *Physical Review A*. **100** (2): 023818. (LA-UR-19-21860 DOI: 10.1103/PhysRevA.100.023818)

*M. Rao, S. J., G. Kumar, A. K. Azad and D. R. Chowdhury. Ultrafast Relaxation of Charge Carriers Induced Switching in Terahertz Metamaterials. 2018. *Journal of Infrared, Millimeter, and Terahertz Waves*. **39** (12): 1211-1220. (LA-UR-18-30111 DOI: 10.1007/s10762-018-0547-6)

*Rodriguez-Lopez, P., W. J. M. Kort-Kamp, D. A. R. Dalvit and L. M. Woods. Nonlocal optical response in topological phase transitions in the graphene family. 2018. *Physical Review Materials*. **2** (1): 014003. (LA-UR-17-30514 DOI: 10.1103/PhysRevMaterials.2.014003)

*Sanders, S., W. J. M. Kort-Kamp, D. A. R. Dalvit and A. Manjavacas. Nanoscale transfer of angular momentum mediated by the Casimir torque. 2019. *Communications Physics*. **2** (1): 71. (LA-UR-18-29153 DOI: 10.1038/s42005-019-0163-3)

*Silva, S. R., A. Rahman, W. de Melo Kort-Kamp, J. J. Rushton, J. Singleton, A. J. Taylor, D. A. R. Dalvit, H. Chen and A. K. Azad. Metasurface-based ultra-lightweight high-gain off-axis flat parabolic reflectarray for microwave beam collimation/focusing. 2019. *Applied Physics Letters*. **9** (1): 18984. (LA-UR-19-22629 DOI: 10.1038/s41598-019-55221-8)

*Szilard, D., W. J. M. Kort-Kamp, F. S. S. Rosa, F. A. Pinheiro and C. Farina. Hysteresis in the spontaneous emission induced by VO phase change. 2019. *Journal of the Optical Society of America B*. **36** (4): C46-C51. (LA-UR-18-30372 DOI: 10.1364/JOSAB.36.000C46)

*Wei, M., X. Hao, A. B. Saxena, W. Qin and S. Xie. Optical Helicity-Manipulated Photocurrents and Photovoltages in Organic Solar Cells. 2018. *The Journal of Physical Chemistry C*. **122** (23): 12566-12571. (LA-UR-18-20268 DOI: 10.1021/acs.jpcc.8b03537)

*Xu, W., L. Xie, J. Zhu, L. Tang, R. Singh, C. Wang, Y. Ma, H. Chen and Y. Ying. Terahertz biosensing with a graphene-metamaterial heterostructure platform. 2019. *Carbon*. **141**: 247-252. (LA-UR-18-29562 DOI: 10.1016/j.carbon.2018.09.050)

*Zhang, J., X. Wei, I. D. Rukhlenko, H. Chen and W. Zhu. Electrically Tunable Metasurface with Independent Frequency and Amplitude Modulations. 2020. *ACS Photonics*. **7** (1): 265-271. (LA-UR-19-29711 DOI: 10.1021/acsphotonics.9b01532)

Reports

Comstock, A. H., S. R. M. Silva, S. Ramani and A. K. Azad. Design and Analysis of a Self-Feed Flat Metasurface Antenna. Unpublished report. (LA-UR-20-25337)

Presentation Slides

Azad, A. K. HARNESSING LIGHT-METASURFACE INTERACTIONS FOR ENABLING TECHNOLOGIES. Presented at *IEEE Research and Applications of Photonics In Defense Conference*,

Miramar Beach, Florida, United States, 2018-08-20 - 2018-08-20. (LA-UR-18-29352)

Azad, A. K. Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces. . (LA-UR-19-20934)

Azad, A. K. LDRD-DR appraisal. . (LA-UR-20-21824)

Azad, A. K., A. E. Cardin, S. R. M. Silva and S. R. Vardeny. Dynamic metasurfaces. . (LA-UR-19-20931)

Azad, A. K. and S. R. Vardeny. LDRD-DR presentation. . (LA-UR-20-21825)

Cardin, A. E. Dynamic Metasurfaces for Advanced Applications. . (LA-UR-21-27661)

Chen, H. Few-Layer THz Metasurfaces for Effective Control of Amplitude, Phase and Polarization States. Presented at *The 4th International Symposium on Microwave/ Terahertz Science and Applications & the 8th International Symposium on Terahertz Nanoscience*, Okayama, Japan, 2017-11-19 - 2017-11-23. (LA-UR-17-30608)

Chen, H. Exotic Properties of Metasurfaces and Their Applications. Presented at *Seminar at University of New Mexico*, Albuquerque, New Mexico, United States, 2018-02-09 - 2018-02-09. (LA-UR-18-21182)

Chen, H. Narrowband Terahertz Bandpass Filters Based on Metasurfaces. Presented at *SPIE Defense + Commercial Sensing*, Orlando, Florida, United States, 2018-04-15 - 2018-04-19. (LA-UR-18-23323)

Chen, H. Hybrid Graphene Metasurfaces for High-Speed Mid-Infrared Modulation. Presented at *The 5th International Conference on Frontiers of Plasmonics (FOP5)*, Nanjing, China, 2018-04-20 - 2018-04-24. (LA-UR-18-23324)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversion. Presented at *The 9th International Symposium on Ultrafast Phenomena and Terahertz Waves (ISUPTW 2018)*, Changsha, China, 2018-04-23 - 2018-04-23. (LA-UR-18-23594)

Chen, H. Hybrid Graphene Metasurface for High-Speed Mid-Infrared Modulation. Presented at *Excited State Process in Electronic and Bio Nanomaterials (ESP-2018)*, Santa Fe, New Mexico, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-25014)

Chen, H. Broadband THz Linear Polarization Rotation and Linear-to-Circular Polarization Conversion Using Metasurfaces. Presented at *OSA Advanced Photonics Congress*, Zurich, Swaziland, 2018-07-02 - 2018-07-05. (LA-UR-18-25397)

Chen, H. Hybrid Graphene Metasurface for High-Speed Mid-Infrared Light Modulation and Single-Pixel Imaging. Presented at *META 2018*, Marseille, France, 2018-06-24 - 2018-06-24. (LA-UR-18-26353)

Chen, H. Achromatic Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. . (LA-UR-19-20968)

Chen, H. Metasurfaces for Manipulating Terahertz Radiation. . (LA-UR-19-25954)

Chen, H. Hybrid Graphene Metasurfaces for High-Speed Mid-Infrared Light Modulation and Single-Pixel Imaging. Presented at *ICMAT 2019*, Singapore, Singapore, 2019-06-24 - 2019-06-24. (LA-UR-19-25955)

Chen, H. Metasurfaces – Achromatic Polarization Conversion and Efficient Optical Modulation. Presented at *Seminar at Argonne National Laboratory*, Lemont, Illinois, United States, 2019-09-11 - 2019-09-11. (LA-UR-19-29185)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversions. Presented at *MTSA 2019*, Busan, Korea, South, 2019-09-30 - 2019-09-30. (LA-UR-19-29968)

Chen, H. Metasurfaces accomplish ultra-broadband optical polarization conversions. Presented at *CLEO Pacific Rim*, Sydney, Australia, 2020-08-03 - 2020-08-03. (LA-UR-20-25943)

Chen, H. Metasurface Broadband Polarization Converters Towards Terahertz Circular Dichroism Spectroscopy. Presented at *IRMMW-THz 2020*, Buffalo, New York, United States, 2020-11-08 - 2020-11-13. (LA-UR-20-30097)

Comstock, A. H., S. R. M. Silva, S. Ramani and A. K. Azad. Design and Analysis of a Self-Feed Flat Metasurface Antenna. . (LA-UR-20-25338)

Cooke, B. J., J. H. Goglio, J. J. Rushton and A. K. Azad. Transition to Mission Applications. . (LA-UR-19-20956)

R. Dalvit, D. A. Nonreciprocal Metasurfaces. . (LA-UR-19-20945)

R. Dalvit, D. A., W. J. de Melo Kort-Kamp and A. K. Azad. Tailoring the Quantum Vacuum via Nonreciprocity and Chirality. Presented at *DARPA QUEST Kickoff Meeting (Remote)*, Los Alamos, New Mexico, United States, 2020-05-15 - 2020-05-15. (LA-UR-20-23407)

de Melo Kort-Kamp, W. J. Shaping photons in nonreciprocal space-time metasurfaces. . (LA-UR-21-28677)

de Melo Kort-Kamp, W. J., D. A. R. Dalvit, S. R. M. Silva and J. J. Rushton. Modeling and Simulation of Static Metasurfaces. . (LA-UR-19-20946)

Saxena, A. B. Nonreciprocity and broken symmetry in photonics: Implications for materials. Presented at *SPIE Optics and Photonics Congress*, San Diego, California, United States, 2018-08-20 - 2018-08-20. (LA-UR-18-27771)

M. Silva, S. R., W. J. de Melo Kort-Kamp, D. A. R. Dalvit, J. J. Rushton, A. K. Azad and H. Chen. Metasurface-based Static Reflectarray Antenna. . (LA-UR-19-20933)

Vardeny, S. R. and A. K. Azad. Testbeds for Active/Dynamic Metamaterial Antennas (ADMA). Presented at *DR Review*, Los Alamos, New Mexico, United States, 2020-02-25 - 2020-02-25. (LA-UR-20-21849)

Posters

Azad, A. K., S. Kramadhati, S. R. M. Silva, N. S. Sirica and H. Chen. Flat Ultrathin Metasurface Parabolic Reflector for THz Applications. . (LA-UR-19-20932)

Cardin, A. E., S. R. M. Silva, S. R. Vardeny, H. Chen and A. K. Azad. Agile Metasurfaces for Beam Manipulation. Presented at *LANL 2019 Student Symposium*, Loa Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27733)

Chen, H., A. D. Tang, S. R. M. Silva, P. L. Cantu, P. Nath and C. Corbella Bagot. Development of an Alvarez metalens in the microwave regime. . (LA-UR-19-20970)

de Melo Kort-Kamp, W. J. Topological Phase Transitions in the Photonic Spin Hall Effect. . (LA-UR-19-20927)

Saxena, A. B. Nonreciprocity and Broken Symmetry. . (LA-UR-19-20944)

Vardeny, S. R. Phase Distribution Surface Controller for Spatio-Temporal Modulated Metasurface Antennas. Presented at *DR Review*, Los Alamos, New Mexico, United States, 2019-02-05 - 2019-02-05. (LA-UR-19-20953)

A Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) Future (U)

Scott Twary
20190167DR

Project Description

Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/CRISPR-associated (Cas) genome engineering is rapidly advancing into all aspects of biology. This work will explore the application of novel CRISPR engineering techniques to regulate stem cell differentiation into muscle and neuron cells. Controlled interactions of these cells will then form functional neuromuscular junctions (NMJs). Effective optimized development of functional NMJs has application to traumatic injury repair, disease therapy, chemical agent testing platforms, and advanced cell biology. Varied genome engineering approaches will create multiple clonal cell lines for in depth characterization of cellular responses to targeted genetic engineering. These lines will be sequenced for genomic modifications, gene regulation responses, gene expression changes, and cellular physical response variation. The integrated analysis will provide a foundational basis for identifying aberrant cell responses to targeted genome engineering. Optimized differentiation of stem cells will provide a capability resource that will enhance biomedical applications, develop chem/bio testing platforms, and advance understanding of genetic responses.

Technical Outcomes

Outcomes of this project include development of multiple Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/CRISPR-associated (Cas) molecular engineering tools applied to human cell lines for differentiation of motor neurons and muscle cells and formation of functional neuromuscular junctions. Multiple computing resources including hardware and software have established a needed capability for identification of the multi-layered challenges analyzing both genomic and transcriptomic data establishing the basis defining the potential consequential secondary modifications arising from directed CRISPR/Cas engineering approaches.

Publications

Journal Articles

Jacobs, L. L. Soil Prokaryotic Cell Size Correlates with Ecosystem Productivity. Submitted to *Soil Biology & Biochemistry*. (LA-UR-19-31347)

Micheva-Viteva, S. N., E. A. Solomon, K. L. Davis-Anderson, S. N. Twary and R. S. Iyer. Global Transcriptome Profile of the Developmental Principles of in vitro iPSC-to-Motor Neuron Differentiation. Submitted to *BMC Neuroscience*. (LA-UR-20-28466)

Pellenz, S., M. Phelps, W. Tang, B. Hovde, R. Sinit, W. Fu, H. Li, E. Chen and R. Monnat. New human chromosomal safe harbor sites for genome engineering with CRISPR/Cas9, TAL effector and homing endonucleases. Submitted to *Human Gene Therapy*. (LA-UR-19-20028)

Sanchez, J. C., S. N. Micheva-Viteva, R. S. Iyer and S. N. Twary. Comprehensive analysis of gene expression from genomic safe harbors in human iPSCs and their differentiated derivatives. Submitted to *Journal of Genetic Engineering and Biotechnology*. (LA-UR-22-22088)

Strickland, J. B., K. L. Davis-Anderson, R. S. Iyer, J. F. Harris and E. A. Solomon. Applications of in vitro neuromuscular junctions for high-throughput screening and disease modeling. Submitted to *Tissue Engineering*. (LA-UR-20-27627)

Strickland, J. B., K. L. Davis-Anderson, S. N. Micheva-Viteva, S. N. Twary, R. S. Iyer, J. F. Harris and E. A. Solomon. Optimization of application-driven development of in vitro neuromuscular junction models. Submitted to *Tissue Engineering, Part B: Reviews*. (LA-UR-21-29377)

Reports

Hovde, B. and J. K. Jurss. Computationally locating off-target effects of CRISPR/Cas9 in human embryonic stem cells. Unpublished report. (LA-UR-19-28097)

Presentation Slides

Davis-Anderson, K. L., S. N. Micheva-Viteva, J. F. Harris, R. S. Iyer and S. N. Twary. CRISPR-Cas9 Reprogramming of Human Stem Cells into Motor Neurons. Presented at *International Society on Stem Cell Research*, virtual, New

Mexico, United States, 2020-06-23 - 2020-06-27. (LA-UR-20-24356)

Harris, J. F. Using Data from Microphysiological systems: Neuromuscular Junction as a Case Study. Presented at *DTRA AI-Med Workshop*, Virtual, District Of Columbia, United States, 2021-11-18 - 2021-11-18. (LA-UR-21-31452)

Hovde, B. and J. K. Jurss. Presentation - Computationally detecting real off-target effects of CRISPR/Cas9 using NGS data. Presented at *Sequencing, Finishing, and Analysis in the Future Meeting*, Santa Fe, New Mexico, United States, 2020-12-01 - 2020-12-03. (LA-UR-20-29659)

Hraber, P. T. Cyberbiosecurity: \xe2\x80\xa8Emerging Research Field \xe2\x80\xa8or Movie-Plot Threat?. Presented at *UNM Computer Science Department Seminar*, Albuquerque, New Mexico, United States, 2019-09-25 - 2019-09-25. (LA-UR-19-29607)

Hraber, P. T. Cyberbiosecurity: \xe2\x80\xa8Emerging Research Field \xe2\x80\xa8or Movie-Plot Threat?. Presented at *UNM Computer Science Department Seminar*, Albuquerque, New Mexico, United States, 2019-09-25 - 2019-09-25. (LA-UR-19-29643)

Posters

Davis-Anderson, K. L., S. N. Micheva-Viteva, E. A. Solomon, J. C. Sanchez, S. N. Twary and R. S. Iyer. CRISPR-Cas9 Directed Reprogramming of Stem Cells into Motor Neurons for Neuromuscular Junction Organoid. Presented at *2019 CBD S&T Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-31218)

Davis-Anderson, K. L., S. N. Micheva-Viteva, J. F. Harris, R. Iyer and S. N. Twary. CRISPR-Cas9 Reprogramming of Human Stem Cells into Motor Neurons. Presented at *Cold Spring Harbor Laboratory: Genome Engineering CRISPR Frontiers*, Virtual, New Mexico, United States, 2020-08-19 - 2020-08-21. (LA-UR-20-26391)

Davis-Anderson, K. L., S. N. Micheva-Viteva, J. F. Harris, R. S. Iyer and S. N. Twary. CRISPR-Cas9 Reprogramming of Human Stem Cells into Motor Neurons. Presented at *International Society on Stem Cell Research*, virtual, New Mexico, United States, 2020-06-23 - 2020-06-27. (LA-UR-20-24355)

Hovde, B. and J. K. Jurss. CRISPR Off-Target Damage Analysis. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27822)

Hovde, B. and J. K. Jurss. Computationally detecting real off-target effects of CRISPR/Cas9 using NGS data. Presented at *Sequencing, Finishing, and Analysis in the Future Meeting*, Santa Fe, New Mexico, United States, 2020-12-01 - 2020-12-03. (LA-UR-20-29658)

Rodriguez, A. M. Motor Neuron Differentiation from Human Embryonic Stem Cells. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-26136)

Sanchez, J. C., E. A. Solomon, K. L. Davis-Anderson, S. N. Micheva-Viteva, R. S. Iyer and S. N. Twary. The conversion of human iPSCs into myocytes via CRISPR/Cas9 technology. Presented at *CSHL Genome Engineering: CRISPR Frontiers*, Cold Spring Harbor, New York, United States, 2020-08-19 - 2020-08-21. (LA-UR-20-26210)

Sanchez, J. C., K. L. Davis-Anderson, E. A. Solomon, R. S. Iyer, S. N. Micheva-Viteva and S. N. Twary. The development of a model for the human neuromuscular junction. Presented at *Cell Symposia: Engineering Organoids and Organs*, San Diego, California, United States, 2019-08-25 - 2019-08-27. (LA-UR-19-28075)

The Remote Elemental, Molecular, and Isotopic Camera (REMICam)

Samuel Clegg
20200770DR

Project Description

The Remote Elemental, Molecular, and Isotopic Camera (REMICam) instrument is a suite of analytical techniques capable of remote chemical, molecular and isotopic analysis in the field. REMICam integrates Laser-Induced Breakdown Spectroscopy (LIBS), Time Resolved Raman Spectroscopy (Raman), Time-Resolved Luminescence Spectroscopy (TRLS), and Visible and Near Infrared Spectroscopy (VisNIR) into a single instrument. REMICam is based on the ChemCam instrument currently operating on the National Aeronautics Space Administration (NASA) Mars Curiosity rover and the SuperCam instrument scheduled to launch on July 30, 2021 on the NASA Perseverance rover. While ChemCam and SuperCam are designed to operate under the reduced martian surface temperature and pressure, REMICam will be the first instrument of its kind to operate under Earth ambient surface temperatures and pressures. This project will discover a new ensemble of signatures and perform advanced quantitative analysis on them. The REMICam instrument will result in revolutionary measurement techniques for many security missions. Finally, forward deployment will be realized by the field demonstrations where REMICam will analyze various chemical, biological, radiological, nuclear, and explosive (CBRNE) samples in the field.

Technical Outcomes

The Remote Elemental, Molecular and Isotopic Camera (REMICam) was successfully assembled using commercial-off-the-shelf parts. The spectrometers were evaluated relative to the scientific performance obtained with the Los Alamos developed spectrometers used on National Aeronautics Space Administration (NASA) SuperCam instrument operating on the Perseverance rover. In summary, REMICam demonstrated that this integrated platform could be used to detect chemical, biological, and explosive materials in support of the national security mission.

Early Detection of Explosive Volcanic Eruptions Using Very High Frequency (VHF) Radiation from Vent Discharges

Sonja Behnke
20190107ER

Project Description

Volcanic ash from an explosive volcanic eruption can rise to aircraft cruising altitudes within 5 minutes of eruption onset, posing a serious threat to aircraft. Thus, timely detection of explosive eruptions and rapid characterization of the resulting ash cloud is a priority for volcano observatories in the United States. The goals of this project are to identify the signal characteristics of a class of volcanic lightning discharges ("vent discharges") that commonly occur in ash plumes and determine how to exploit these characteristics in a radio frequency-based volcanic eruption monitoring system. This work will advance the state of the art of volcano monitoring and address gaps in current methods. In addition, the knowledge gained about the signal characteristics of vent discharges and the methods to discriminate them from other types of lightning and other radio frequency transients can be applied to mission areas that are of interest to the National Counter Proliferation Center. For example, vent discharges are similar to electrical discharges produced by chemical explosions; the scientific understanding gained from this work can help inform a science-based simulation framework to model the characteristics and signatures of a non-nuclear test device, from early detonation to late time combustion.

Publications

Journal Articles

. E. H. *. S. S. *. I. M. *. M. D. Behnke, S. A. and S. A. Behnke. Radio Frequency Characteristics of Volcanic Lightning and Vent Discharges. 2021. *Journal of Geophysical Research: Atmospheres*. **126 (18): e2020JD034495. (LA-UR-20-30282 DOI: 10.1029/2020JD034495)

Behnke, S. A., H. Edens, J. P. Theiler, D. J. Swanson, S. Senay, A. R. Van Eaton, M. Iguchi and D. Miki. Discriminating Types of Volcanic Electrical Activity: Toward an Eruption Detection Algorithm. Submitted to *Geophysical Research Letters*. (LA-UR-21-29317)

B. S. *. E. H. *. T. R. Haley, S. *., S. Haley and S. Behnke. Observations Show Charge Density of Volcanic Plumes is Higher Than Thunderstorms. 2021. *Journal of Geophysical Research: Atmospheres*. **126** (19): e2021JD035404. (LA-UR-21-25344 DOI: 10.1029/2021JD035404)

Presentation Slides

Behnke, S. A., H. E. Edens, J. P. Theiler, D. J. Swanson, S. Senay, M. Iguchi and D. Miki. A Method for Discriminating Types of Volcanic Electrical Activity. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31924)

Posters

Behnke, S. A., H. E. Edens, S. Senay, J. B. Johnson, K. B. Eack, M. P. Caffrey, J. P. Theiler, A. R. Van Eaton, D. J. Schneider, M. Iguchi and D. Miki. Early Detection of Explosive Volcanic Eruptions Using VHF Radiation from Vent Discharges. Presented at *American Geophysical Union Fall Meeting 2019*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32189)

Behnke, S. A., H. E. Edens and J. P. Theiler. Vent Discharges Produced by Explosive Volcanic Eruptions: Characteristics, Signatures, and Volcano Monitoring Applications. Presented at *American Geophysical Union Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31441)

Haley, S. L., S. A. Behnke, H. E. Edens and R. J. Thomas. Exploring Properties of Volcanic Lightning using Electric Field Change Measurements and 3D Lightning Mapping Data. Presented at *American Geophysical Union Fall Meeting 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29374)

Swanson, D. J., S. A. Behnke, C. M. Smith and A. R. Van Eaton. Examining the Relationship Between Electrical Activity and Jet Velocity During Explosive Volcanic Eruptions at Sakurajima Volcano. Presented at *American Geophysical Union Fall Meeting 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-01. (LA-UR-20-29343)

Unveiling the Heating and Acceleration of Solar Wind by "Touching" the Sun with the Parker Solar Probe

John Steinberg
20200270ER

Project Description

This project aims at understanding the origin of Solar Wind (SW), a plasma gas that is heated and accelerated away from the Sun and fills the solar system. This is a fundamental question for understanding of the space weather and it could have a major impact on understanding how SW impacts Earth's nearby space environment known as the magnetosphere. This project brings together observations, data analysis, theory, and numerical modeling of SW plasma particles and magnetic fields. It builds capabilities in space plasma and field detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Publications

Journal Articles

Arnold, H., J. F. Drake, M. Swisdak, F. Guo, J. Dahlin, Q. Zhang, J. Karpen and C. R. Devore. Slow Shock Formation Upstream of Reconnecting Current Sheets. Submitted to *Astrophysical Journal*. (LA-UR-21-27254)

Du, S., H. Li, X. Fu, Z. Gan and S. Li. Magnetic Energy Conversion in MHD: Curvature Relaxation and Perpendicular Expansion of Magnetic Fields. Submitted to *Astrophysical Journal*. (LA-UR-21-30494)

Gan, Z., H. Li, X. Fu and S. Du. On the Existence of Fast Modes in the Compressible Magnetohydrodynamic Turbulence. Submitted to *Astrophysical Journal Letters*. (LA-UR-21-31374)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

*Lazarian, A., G. L. Eyink, A. Jafari, G. Kowal, H. Li, S. Xu and E. T. Vishniac. 3D turbulent reconnection: Theory, tests, and astrophysical implications. 2020. *Physics of Plasmas*. **27** (1): 12305. (LA-UR-20-28591 DOI: 10.1063/1.5110603)

Lazarian, A., O. Khabarova, S. Xu and F. Guo. Violation of Flux Freezing, Turbulent Magnetic Reconnection and induced Particle Acceleration. Submitted to *Review of Modern Plasma Physics*. (LA-UR-21-27253)

Li, H. Fast Magnetic Reconnection with Turbulence in High Lundquist Number Limit. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-24765)

*Seo, B., P. Wongwaitayakornkul, M. A. Haw, R. S. Marshall, H. Li and P. M. Bellan. Determination of a macro- to micro-scale progression leading to a magnetized plasma disruption. 2020. *Physics of Plasmas*. **27** (2): 22109. (LA-UR-20-28589 DOI: 10.1063/1.5140348)

Yu, F., X. Kong, F. Guo, Y. Chen and J. Giacalone. Double-power-law feature in the energy spectra of energetic particles accelerated at coronal shocks. Submitted to *Astrophysical Journal*. (LA-UR-21-27255)

Presentation Slides

Conrad, E. K., J. T. Steinberg, R. M. Skoug, J. M. Broll, S. Du, H. Li, X. Fu and Z. Gan. Solar Wind Density Variability and Pressure Balance Near the Sun. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31868)

Du, S., H. Li, X. Fu, Z. Gan, F. Guo and X. Li. Magnetic Energy Conversion in Magnetically Dominated Systems and Implications for Particle Energization Processes. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31939)

Li, H. 3D Turbulence with Global Reconnection. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-28062)

Li, H. Turbulent Dynamo Modeling and Experiments using HED Plasmas. Presented at *AAPPS-DPP2020 On-line E-conference*, Pohang, Korea, South, 2020-10-26 - 2020-10-26. (LA-UR-20-28587)

Li, H. IC Project: Heating and Acceleration of Solar Wind by Parametric Decay Instability Mediated Turbulence. . (LA-UR-21-23434)

Li, H. Compressible MHD Turbulence and Implications for Solar Wind Turbulent Density Variations Measured by Parker Solar Probe. Presented at *Fundamentals of compressible*

turbulence: recent advances and open questions, college station, Texas, United States, 2021-05-20 - 2021-05-21. (LA-UR-21-24830)

Li, H. Compressible MHD Turbulence and Implications for Solar Wind Turbulent Density Variations Measured by Parker Solar Probe. Presented at *The 2021 Midwest Magnetic Field Workshop*, Madison, Wisconsin, United States, 2021-06-14 - 2021-06-14. (LA-UR-21-25650)

Li, H. On the Existence of Finite Frequency Fast Modes in the Compressible MHD Turbulence. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-31375)

Li, H. Magnetic Energy Conversion in Magnetically Dominated Systems and Implications for Particle Energization Processes. Presented at *63rd Annual Meeting of the APS Division of Plasma Physics*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-08. (LA-UR-21-31376)

Li, H. and X. Fu. Heating of Heavy Ions in Low-beta Compressible Turbulence. Presented at *2019 AGU Fall Meeting*, san francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-20-28060)

Li, H. and X. Fu. Compressible Turbulence in the Solar Wind near the Sun. Presented at *19th AIAC Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-28061)

Deep Learning Interferometric Synthetic-Aperture Radar

Bertrand Rouet-Leduc
20200278ER

Project Description

Small ground deformations are associated with a variety of phenomena of critical importance: slow earthquakes, earthquakes precursors, aquifer levels variations, oil and gas extraction, water injection for geothermal applications, carbon dioxide sequestration, underground explosions, underground construction. Recent deployments of satellites for advanced radar imagery has enabled the unprecedented ability to monitor ground deformation globally. However, ground deformation maps acquired from radar interferometry suffers from very high levels of noise due to atmospheric disturbances and current state-of-the-art analysis relies on time consuming expert interpretation, preventing global detection of small deformations. We are developing a deep learning artificial intelligence specifically built to extract ground deformation signals of interest in interferometric synthetic aperture radar (InSAR) data. Our technology will unlock the ability to automatically monitor all deformations of interest globally, including small and slow deformations. The work will place the Laboratory at the forefront of underground deformation signature detection and induced earthquake mitigation. The approach we are developing also has application to ground based nuclear explosion monitoring, where even minute surface deformation signatures will become detectable. There will be applications to Fossil Energy, Carbon Sequestration and Geothermal problems, and to ongoing work funded by the Office of Science on deformation associated with faulting.

Publications

Journal Articles

Hulbert, C. L., B. P. G. Rouet-Leduc, P. A. Johnson and R. Jolivet. Automatic Tremor Location with Neural Network Interpretation. Submitted to *Geophysical Research Letters*. (LA-UR-20-22490)

Hulbert, C. L., B. P. G. Rouet-Leduc, P. A. Johnson and R. Jolivet. An exponential build-up in seismic energy suggests a months-long nucleation of slow slip in Cascadia. Submitted to *Nature Communications*. (LA-UR-19-29448)

Johnson, P. A. and B. P. G. Rouet-Leduc. Laboratory Earthquake Forecasting: A Machine Learning Competition. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-28829)

Licciardi, A., Q. Bletery, B. P. G. Rouet-Leduc, J. Ampuero and K. Juhel. Instantaneous Tracking of Earthquake Growth Using Prompt Elasto-Gravity Signals and Deep Learning. Submitted to *Nature*. (LA-UR-21-30873)

*Rouet-Leduc, B., C. Hulbert, I. W. McBrearty and P. A. Johnson. Probing Slow Earthquakes With Deep Learning. 2020. *Geophysical Research Letters*. **47** (4). (LA-UR-19-27444 DOI: 10.1029/2019GL085870)

Books/Chapters

G. Rouet-Leduc, B. P., C. X. Ren, C. L. Hulbert and P. A. Johnson. Machine learning and fault rupture: A review. (LA-UR-20-28827)

Reports

Angermeier, W., C. Barros, I. D. Dumitru, M. C. Holmes, J. R. Howard, S. R. Johnstun, G. B. King, J. T. Lindbloom, N. P. Lordi, A. Luu, S. E. Martinez, J. N. McBride, E. S. Nelluvelil, K. T. O'Dell, H. R. Pace, N. A. Poole, A. Ramkumar, S. M. Riedel, L. Singh, S. R. Venkat, D. A. Weatherred, J. Y. Wei, K. A. York, F. Yousuf, M. T. Andrews, D. M. Israel and J. A. Kulesza. Final Reports of the 2021 Los Alamos National Laboratory Computational Physics Student Summer Workshop. Unpublished report. (LA-UR-21-28941)

Presentation Slides

Ren, C. X., B. P. G. Rouet-Leduc, S. R. Venkat and K. T. O'Dell. Deep Learning for Satellite Imagery: Modelling Atmospheric Effects. . (LA-UR-21-27903)

The Role of Defects in Solid State Detonation Kinetics

Pamela Bowlan
20200311ER

Project Description

After decades of modeling and experiments, the physical mechanism by which a detonation occurs remains a mystery. Of particular interest to the Laboratory and national security are secondary solid explosives because of their relative insensitivity, but this lack of understanding seriously impedes our ability to predict their performance and safety. The reason for this uncertainty is not understanding how an impulse, such as an increase in temperature or pressure, leads to the fast chemistry that makes up a detonation wave. As a result, models have to infer the needed chemical rate equations from indirect measurements, which constrains the range of phenomena that can be predicted by a single model. The purpose of the work proposed here is to directly measure the kinetics of detonation in secondary explosives taking the nanosecond(ns)-time-scale loss of crystallinity to be the relevant progress variable. Our unique experimental approach can lead to a breakthrough study in explosives science that reveals the rate limiting step in detonation and an improved set of kinetics equations that can be implemented in reactive burn models, broadening the scope of phenomena that can be accurately predicted.

Publications

Journal Articles

Bowlan, P. R., B. F. Henson, L. B. Smilowitz, N. A. Suvorova and D. M. (. Oschwald. Acceleration of thermal decomposition near the melting point in organic molecular crystals. Submitted to *Journal of Chemical Physics*. (LA-UR-20-22788)

Bowlan, P. R., N. A. Suvorova, D. K. Remelius, L. B. Smilowitz and B. F. Henson. Acceleration of thermal decomposition near the melting point in organic molecular crystals. Submitted to *Journal of Applied Physics*. (LA-UR-20-29950)

Bowlan, P. R., N. A. Suvorova, D. K. Remelius, L. B. Smilowitz and B. F. Henson. Tracking thermal decomposition chemistry in secondary solid explosives with x-ray diffraction. Submitted to *Journal of Physical Chemistry A*. (LA-UR-21-25685)

Bowlan, P. R., N. A. Suvorova, D. K. Remelius, L. B. Smilowitz and B. Henson. Tracking thermal decomposition chemistry in organic crystalline solids with x-ray diffraction. Submitted to *Journal of Physical Chemistry A*. (LA-UR-21-31193)

Presentation Slides

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius and N. A. Suvorova. Time resolving the loss of crystallinity during detonation in a solid explosive. Presented at *APS March Meeting*, virtual meeting, New Mexico, United States, 2021-03-15 - 2021-03-15. (LA-UR-21-22332)

Parallel Magnetic Resonance Imaging with a Multichannel Radio-frequency Atomic Magnetometer

Young Jin Kim
20200393ER

Project Description

The goals of this project are (1) to construct a new ultra-low field (ULF) magnetic resonance imaging (MRI) system based on a novel technique of a multichannel single-cell radio-frequency (RF) atomic magnetometer (AM) with multiple flux transformers (FTs) and demonstrate high sensitivities in each sensing channel in an unshielded environment; (2) to perform feasibility proof by initial parallel MRI experiments using a water phantom; (3) to demonstrate its application in accelerated MRI measurements of human subject such as a human brain, hand, and spine, which will be an exciting event for the biomedical community. This project will lead to cost-effectiveness and image acceleration, which will be an important revolution and a major breakthrough in biomagnetic diagnostics leading to new medical applications. In addition, it will put Los Alamos in the leading position in novel imaging applications, including in medical imaging and nuclear quadrupole resonance (NQR) imaging for explosive detection, and will be a unique capability in multichannel RF AM.

Publications

Journal Articles

*Kim, Y. J. and I. M. Savukov. Parallel high-frequency magnetic sensing with an array of flux transformers and multi-channel optically pumped magnetometer for hand MRI application. 2020. *Journal of Applied Physics*. **128** (15): 154503. (LA-UR-20-24994 DOI: 10.1063/5.0021284)

Savukov, I. M. and Y. J. Kim. Investigation of magnetic noise from conductive shields in the 10–300 kHzfrequency range. Submitted to *Journal of Applied Physics*. (LA-UR-20-27307)

Presentation Slides

Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)

Kim, Y. J., I. M. Savukov and S. G. Newman. Magnetic Resonance Imaging (MRI) with a Multichannel Optically Pumped Magnetometer. Presented at *APS March Meeting 2022*, CHICAGO, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-22078)

Kim, Y. J. and I. M. Savukov. Development of a multichannel atomic magnetometer for parallel magnetic resonance imaging. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21897)

Savukov, I. M. and Y. J. Kim. Broadband Ultra-sensitive Adiabatic Magnetometer. Presented at *SAS 2012*, Virtual, Sweden, 2021-08-23 - 2021-08-25. (LA-UR-21-27516)

Savukov, I. M. and Y. J. Kim. Multi-channel radio-frequency optically pumped magnetometers and their applications in MRI. Presented at *Virtual WOMP meeting*, Berlin, Germany, 2021-10-04 - 2021-10-05. (LA-UR-21-29802)

Posters

Savukov, I. M. and Y. J. Kim. Development of multi-channel parallel atomic magnetometer MRI. Presented at *Practical Applications of NMR in Industry Conference (PANIC 2020) --Virtual meeting*, Los Alamos, New Mexico, United States, 2020-10-19 - 2020-10-22. (LA-UR-20-27922)

Broadband Terahertz Circular Dichroism Spectroscopy

Houtong Chen
20200419ER

Project Description

Although the richness of terahertz (THz, or far-infrared) spectral fingerprints in large biomolecules makes THz circular dichroism (THz-CD) spectroscopy an extremely important tool to detect functionally relevant dynamic modes, currently there is no existence of any THz-CD system for practical use due to the lack of high-performance THz circular polarization modulators. We tackle this long-standing challenge by taking advantage of our recent patent-pending metasurface technology, which allows us to develop, for the first time in the world, a broadband THz-CD spectrometer and measure the rich signature of global dynamic modes and conformation changes within large chiral biomolecules. The success of the proposed work, including the instrumentation itself and the corresponding scientific discoveries utilizing this instrument, will pave an avenue to solve problems in biochemistry, drug discovery, and food research laboratories and industries. Upon the completion of this project, the anticipated deliverables include: a) A set of high-performance, broadband THz metasurface circular polarization modulators cover the entire THz band; b) A THz-CD spectrometer for measurements of chiral biomolecules and biomaterials; c) A set of THz CD spectroscopy data first ever for a variety of biomolecules related to molecular structures and functions.

Publications

Journal Articles

*Chang, C., Z. Zhao, D. Li, A. J. Taylor, S. Fan and H. Chen. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. 2019. *Physical Review Letters*. **123** (23): 237401. (LA-UR-18-31108 DOI: 10.1103/PhysRevLett.123.237401)

Chen, H., S. R. M. Silva, C. Corbella, A. D. Tang, P. Nath and A. K. Azad. Microwave Metasurface-Based Alvarez Lens. Submitted to *Applied Physics Letters*. (LA-UR-20-30096)

Chen, H., Y. Zhang, T. Wang, J. Guo and X. Wang. High efficiency spatial terahertz modulator. Submitted to *Journal of Applied Physics*. (LA-UR-21-30748)

Chen, H., Z. Zhao, D. Li, A. J. Taylor, S. Fan and C. Chang. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. Submitted to *Physical Review Letters*. (LA-UR-19-29771)

Presentation Slides

Chen, H. Metasurfaces accomplish ultra-broadband optical polarization conversions. Presented at *CLEO Pacific Rim*, Sydney, Australia, 2020-08-03 - 2020-08-03. (LA-UR-20-25943)

Chen, H. Metasurface Broadband Polarization Converters Towards Terahertz Circular Dichroism Spectroscopy. Presented at *IRMMW-THz 2020*, Buffalo, New York, United States, 2020-11-08 - 2020-11-13. (LA-UR-20-30097)

A New Approach to Predict Toxicity of Small Molecule Toxins

Hau Nguyen
20210172ER

Project Description

Biochemical agents, and toxin molecules in particular, pose one of the greatest threats to our national security, as shown by multiple attempts in recent decades to poison government officials in the United States and Great Britain. Devising effective means to identify and screen for toxins from environmental samples is thus a crucial component of modern national security measures. Unlike radiological threat agents, toxins appear inert in the environment, and only display their functionality once ingested or absorbed by an organism, making them a dangerously insidious form of potential terrorism that requires advanced identification measures. By developing analytical methods that can rapidly identify toxins by their molecular structure, and thus avoid the need for testing functionality on living systems, we will be able to screen environments for toxin molecules in high-throughput and identify the expected toxicity of an environment. This research also has the potential to inform the development of novel therapeutics with similar molecular structures and functionality. Thus our methods will benefit national security as well as development of new therapeutics for medical treatment.

Publications

Journal Articles

B. Nguyen, H. T., G. S. Waldo and T. C. Terwilliger. Engineering an Efficient and Bright Split Corynactis Californica Green Fluorescent Protein. Submitted to *Scientific Reports*. (LA-UR-21-25224)

B. Nguyen, H. T., L. Huynh, G. Gupta, J. Vel\xc3\xa1squez, R. Rabara and S. Basu. Rational design of antimicrobial peptides targeting Gram-negative bacteria. Submitted to *Computational Biology and Chemistry*. (LA-UR-21-20035)

Presentation Slides

Miner, J. C. Combined experimental / computational characterization of small biotoxin structures. . (LA-UR-21-22118)

Miner, J. C. Characterizing RNA molecules through high-performance computing. . (LA-UR-21-26081)

Long-lived Fauna as Tracers of Anthropogenic Radionuclides

Cyler Conrad
20210220ER

Project Description

Historic, legacy radionuclide records from the era of above ground nuclear testing are difficult to capture and analyze. Using long-lived animal skeletons curated in museum collections, specifically tortoises and turtles, we plan to analyze radionuclides which are deposited on a yearly basis within tortoise shell to understand anthropogenic radionuclide incorporation into this animal and tissue type from the Trinity Test Site, Nevada Test Site, in Kazakhstan and in the Galapagos. Our challenge is to find new ways to track radionuclides in the environment, especially to further the goals of nuclear forensics and non-proliferation programs within the Department of Energy and other associated federal agencies. If we are successful in identifying and analyzing annual records of radionuclides from tortoise/turtle shell tissue, we expect that this technique will be valuable in aiding radionuclide identification from nuclear testing or processing facilities/activities, and clandestine passive collecting approaches.

Publications

Presentation Slides

Conrad, C. N., A. M. Wende, J. D. Inglis, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, S. M. Gaukler, J. J. Whicker, W. T. Aguilera, J. P. Gibbs and B. Wolf. Long-lived Fauna as Tracers of Anthropogenic Radionuclides. . (LA-UR-20-29525)

Conrad, C. N., A. M. Wende, J. D. Inglis, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, S. M. Gaukler, J. J. Whicker, W. Tapia Aguilera, J. Gibbs and B. Wolf. Tracing the legacy of anthropogenic radionuclides from 20th Century nuclear testing in desert tortoises (Gopherus agassizi) at the Nevada Test Site. Presented at *Desert Tortoise Council*, Tuscon, Arizona, United States, 2021-02-16 - 2021-02-16. (LA-UR-21-21186)

Conrad, C. N., J. D. Inglis, N. Mukundan, A. M. Wende, T. J. Tenner, K. N. Wurth, B. E. Naes, J. M. Fair, E. A. Middlebrook, S. M. Gaukler, J. J. Whicker, W. T. Aguilera, J. P. Gibbs and B. Wolf. Tortoises and Turtles as Passive Collectors of Anthropogenic Radionuclides from Nuclear Testing and Production Activities. Presented at *Turtle Survival Alliance*, Charleston, South Carolina, United States, 2021-08-13 - 2021-08-13. (LA-UR-21-27883)

Inglis, J. D. Analysis of Turtle and Tortoise Scutes can Provide a Time-Constrained Record of Radionuclide Releases into the Environment. Presented at *International Conference on Methods and Applications of Radioanalytical Chemistry (MARC)*, kailua-Kona, Hawaii, United States, 2022-04-04 - 2022-04-04. (LA-UR-22-22272)

Identification of Gamma Radiation Enabled by Semi-conductive Nanocrystalline Materials

Amanda Graff
20210253ER

Project Description

The current limitations of nuclear material detection and identification can be viewed largely as a function of the sensing materials used in radiation detectors. Not only have commonly used materials have been technologically stagnant for decades, they either are expensive to produce on a large scale or require cryogenic temperatures for efficient operations. Our research will lay the groundwork for the development of radiation detectors that address current shortcomings. Our goal is to produce radiation detectors not only capable of quickly detecting and identifying radioactive material without cumbersome cooling equipment, but also at a lower cost than state-of-the-art commercial detectors. Successful execution of this project will have a direct impact on every activity that is dependent on fast and accurate identification of not only special nuclear material (SNM). Such activities include nonproliferation, counter-proliferation, and emergency response efforts.

Most Sensitive Optical Quantum Sensor

Young Jin Kim
20210254ER

Project Description

This project will result in a new high-frequency optical quantum sensor (OQS) with sensitivity reaching the fundamental quantum limit, beyond the capability of current technology in magnetic field detection. The new sensor technology would address the sensor sensitivity limitation problem in many existing high-precision magnetic field measurements by improving the sensitivity of the best available commercial magnetic sensors by more than two orders of magnitude. The advanced OQS will contribute to the grand scientific challenge of discovering new physics beyond the Standard Model of particle physics, supporting the Laboratory's fundamental science mission and Nuclear and Particle Futures science pillar. This project will also provide opportunities to develop the talent pipeline and technology supporting the Laboratory's national security mission.

Publications

Journal Articles

Savukov, I. M. and Y. J. Kim. Broadband Ultra-sensitive Adiabatic Magnetometer. Submitted to *IEEE Sensors*. (LA-UR-21-24891)

Presentation Slides

Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)

Atom Interferometry without Coherence

Malcolm Boshier
20210301ER

Project Description

The National Quantum Initiative recognizes the importance to the Nation of quantum information technologies such as quantum sensing. We have developed a rotation sensor that will eventually enable accurate navigation when a Global Positioning System (GPS) is denied or unavailable. That is a pressing challenge facing both the Defense and Intelligence communities. The sensor can also be configured to measure gravitational fields, which has applications to nonproliferation. This project will use a protocol originally developed for quantum computing to enhance the performance of our sensor beyond the usual boundaries imposed by noise, which will have high impact on the areas above.

Publications

Journal Articles

Zurek, W. H. Quantum Theory of the Classical: Einselection, Envariance, and Quantum Darwinism. Submitted to *Entropy*. (LA-UR-21-31822)

Presentation Slides

Calder, C. M. Automation and Machine Learning for Robust and Self-Tuning Magneto-Optical Traps. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2021-08-03 - 2021-08-03. (LA-UR-21-27580)

Calder, C. M. Automation and Machine Learning for Robust and Self-Tuning Magneto-Optical Traps. Presented at *EERE AMO Internships Summer Presentation*, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-27748)

Girolami, D., A. Touil, B. Yan, S. Deffner and W. H. Zurek. Quantitative limits to quantum correlations in many-body systems: a signature of classical objectivity. Presented at *American Physical Society (APS) March Meeting*, Chicago, Illinois, United States, 2022-03-14 - 2022-03-18. (LA-UR-22-21970)

Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

Zurek, W. H. Information Scrambling, Loschmidt Echo, and Decoherence. . (LA-UR-21-29934)

Gleaming the Cube: Advanced Focal Planes for Optimal Acquisition of Spectral Images

John Bowlan
20210306ER

Project Description

A hyperspectral image (HSI or data cube) is an image where hundreds of spectral channels are acquired for every pixel. It is a powerful remote sensing technique that can passively identify the spectral signatures of materials from up to 100's of km away. Current state-of-the art HSI systems make inefficient use of available light because the same acquisition settings must be used for all areas of an image. We will develop a prototype image sensor using a novel focal plane array (FPA) design that is optimized for the acquisition of hyperspectral images. We expect significant improvements over the current state-of-the-art in frame-rate and signal-to-noise (SNR), while avoiding the traditional engineering trade-offs against spectral resolution. These gains are achieved by allowing each pixel to adapt to the dynamic characteristics the scene. Our proposed design exploits recent advances in infrared focal plane arrays, and aims to enable the application of passive spectral imaging to scenarios where it is not currently practical, such as handheld operation and acquisition of moving objects. The improved sensitivity will also enable the detection of entirely new classes of spectral signatures that are beyond the capabilities of today's technology.

Publications

Conference Papers

Thurmond, K. D. and J. M. Bowlan. Analysis of Phase-Controlled Fourier Transform Spectroscopy for Remote Sensing Applications. Presented at *optica optical sensor and sensing congress*. (Vancouver, Canada, 2022-07-11 - 2022-07-15). (LA-UR-22-22468)

Whispering-Gallery-Resonator Beads for Rapid and Sensitive Chemical Threat Detection

Laura Lilley
20210367ER

Project Description

Chemical threat and toxic industrial agents pose a threat to national security. Fortunately, outside of World War I there have been limited modern examples of chemical agent (clandestine or otherwise) use. There have, however, been several modern examples of devastating toxic industrial agent accidents including the Seveso disaster in 1976 and the Bhopal India release in 1989. The global expansion of commodity and pharmaceutical industries greatly expands access to these agents and presents a need for technological advancement in chemical threat detection/identification. We will address CBRNE (Chemical, Biological, Radiological, Nuclear, and high yield Explosives) threat reduction efforts by improving detection strategies for chemical signatures. This research focuses on a new fieldable detection method with unparalleled gas detection multiplexing. Whispering gallery mode resonator microspheres (functionalized for chemical threat agent detection) offer a potent solution to challenges currently present in the detection of chemical threats in highly complex mixtures. Further, we are building a robust signal processing and spectral library infrastructure that will enable this technology to be deployable. Facilitating rapid, sensitive, and selective multiplexed detection methods for such agents serves the dual role of providing a proof-of-concept while addressing the national and international need.

Publications

Journal Articles

Paulus, B. C., J. K. Banh, K. D. Rector, B. Stein and L. M. Lilley. Continuous Flow Measurements of Whispering Gallery Mode Spectra for Characterization of Microspherical Resonators and Their Local Environment. Submitted to *Analytical Chemistry*. (LA-UR-21-30848)

Presentation Slides

Lilley, L. M. Journey to the National Laboratory. . (LA-UR-20-30040)

Posters

Paulus, B. C., J. K. Banh, K. D. Lenz, K. D. Rector, B. Stein and L. M. Lilley. Continuous Flow Measurements of Whispering Gallery Mode Spectra for Characterization of Microsphere Resonators and their Local Environment. Presented at *ACS Spring 2022 Bonding Through Chemistry*, San Diego, California, United States, 2022-03-20 - 2022-03-24. (LA-UR-22-22227)

Dark Field Proton Radiography

Matthew Freeman
20210419ER

Project Description

Proton radiography (pRAD) typically operates in a very high density regime, aquiring 21 imaging frames on a 200-nanseconds (ns) timescale, while other imaging modalities are either well suited for visualizing thinner objects, or do not have the temporal capabilities of pRad. This development seeks to broaden the applicability of pRad by visualizing thinner processes on a fast timescale, and to improve the workflow of the pRad facility by streamlining what is now a time consuming process: adjusting collimator (transmission) settings. The goal of this project is to evaluate a very subtle, but fast system, such as the mixing of high-Atwood number gases under pressure loading. It is expected that we will optimize this system to be better able to visualize such low-contrast processes, and that we will streamline the workflow at pRad to allow for quicker shot-to-shot turnaround through the automated, blast-proof collimator assembly that we will provide.

Publications

Journal Articles

Broder, B. A., E. F. Aulwes, M. A. Espy, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. S. Freeman. A TOPAS model for lens-based proton radiography. Submitted to *Medical Physics*. (LA-UR-21-28343)

Broder, B. A., E. F. Aulwes, M. A. Espy, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. S. Freeman. A TOPAS model for lens-based proton radiography. Submitted to *Physics in Medicine and Biology*. (LA-UR-22-20784)

Presentation Slides

Freeman, M. S. Charged Particle Radiography as an HED Diagnostic. Presented at *41stInternational Workshop on High Energy-Density Physics with Intense Laser Beams*, Virtual, New Mexico, United States, 2021-02-01 - 2021-02-01. (LA-UR-21-21038)

Posters

Broder, B. A. and M. S. Freeman. ASSESSMENT OF CLINICAL TO HIGH ENERGY PROTON RADIOGRAPHY VIABILITY USING TOPAS. Presented at *American Association of Physicists in Medicine Annual Meeting*, Virtual, New Mexico, United States, 2021-07-28 - 2021-07-28. (LA-UR-21-27482)

Listening for Rock Coatings on Mars: Using Acoustic Signals from Laser-Induced Breakdown Spectroscopy

Nina Lanza
20210424ER

Project Description

Rock coatings are a key place in which to search for signs of life on Mars, which is a major goal of the National Aeronautics and Space Administration (NASA) Perseverance Mars rover. The Los Alamos led SuperCam instrument suite onboard Perseverance is highly suited for the study of rock coatings because it includes both a laser-induced breakdown spectroscopy (LIBS) instrument and a microphone to record the zapping sound of LIBS laser sparks. By examining both the chemical and acoustic signals obtained by LIBS, the presence and nature of a rock coating may be positively identified. The goal of this work is to identify rock coatings in a Mars-like environment using the acoustic signals (zapping sounds) from laser-induced breakdown spectroscopy analyses. The proposed work will position Los Alamos at the forefront of an emerging field of study by laying the foundation for a new type of analysis for natural rocks, as well as building fundamental knowledge about LIBS acoustics and sound propagation on Mars.

Publications

Conference Papers

Larmat, C., E. R. Dauson, A. L. Reyes-Newell, A. M. Ollila, J. A. Ten Cate, B. Chide, N. L. Lanza and R. C. Wiens. Using Laboratory LIBS Acoustics Experiments to Elucidate SuperCam Microphone Data on Mars.. Presented at *53rd Lunar and Planetary Science Conference*. (Woodlands, Texas, United States, 2022-03-07 - 2022-03-11). (LA-UR-22-20251)

Presentation Slides

Dauson, E. R. Acoustic signals from laser-induced breakdown spectroscopy: Listening for coatings on Martian rocks. . (LA-UR-20-30175)

Rolland, L., C. Larmat, O. Karatekin, A. Spiga, E. Samson, B. Fernando, G. Sainton and P. Lognonn\xc3\xa9. Sonic Booms from Atmospheric Entries. Presented at *2021 AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31936)

Rolland, L., C. Larmat and O. Karatekin. Sonic Boom and Impact Acoustics on Mars and Earth. Presented at *22th InSight Science Team Meeting*, Online, New Mexico, United States, 2021-10-25 - 2021-10-29. (LA-UR-21-30644)

Rolland, L., O. Karatekin and C. Larmat. Sonic Booms from spacecraft entries, a Mars/Earth perspective. Presented at *InSight Science Team Meeting 21-2021*, online, New Mexico, United States, 2021-06-28 - 2021-07-01. (LA-UR-21-26087)

Posters

Larmat, C., E. R. Dauson, A. L. Reyes-Newell, A. M. Ollila, J. A. Ten Cate, B. Chide, N. L. Lanza and R. C. Wiens. USING LABORATORY LIBS ACOUSTICS EXPERIMENTS TO ELUCIDATE SUPERCAM MICROPHONE DATA ON MARS.. Presented at *53th Lunar and Planetary Science Conference*, Online, New Mexico, United States, 2022-03-07 - 2022-03-11. (LA-UR-22-21971)

High Dynamic Range Neutron Detector for Pulsed Applications

Markus Hehlen
20210431ER

Project Description

A short pulse of neutrons arriving at a remote detector is a highly valuable signature of a nuclear event as it carries information about the intensity, dynamics, and energetics of the source. The remote measurement of a short neutron pulse is essential to the Space-based Nuclear Detonation Detection (SNDD) program supporting DOE's treaty verification mission. It is also a key capability for the Neutron Diagnosed Subcritical Experiment (NDSE) and Enhanced Capabilities for Subcritical Experiments (ECSE) programs in support of the Stockpile Stewardship mission. Traditional helium-3 (He-3) tubes suffer from a limited dynamic range. We aim to overcome this limitation by exploring and demonstrating a new type of neutron detector that is expected to have a ~5000× higher dynamic range than He-3 detectors for the same detection efficiency. The detector combines a composite scintillator with a high-dynamic range readout of silicon photomultipliers. We will explore and develop a high dynamic range calibration scheme, parallel readout of silicon photomultipliers, and an optically transparent composite scintillator. We expect these research themes to yield several publications and new patent applications. The successful completion of the proposed work will establish the multi-disciplinary knowledge base that will enable us to propose a subsequent application-specific detector development.

Publications

Journal Articles

Wiggins, B. W., M. P. Hehlen, R. O. Nelson and C. G. Richards. Optical transport simulations in radiation damaged scintillating particle composite systems. Submitted to *Journal of Applied Physics*. (LA-UR-19-29565)

Conference Papers

Taylor, C. E. STUDY FOR ALTERNATIVE CAVITY WALL AND INDUCTIVE INSERT MATERIAL. Presented at *IPAC*. (Campinas, Brazil, 2021-05-25 - 2021-05-25). (LA-UR-21-25753)

Presentation Slides

Taylor, C. E., J. T. M. Lyles, C. Chen, J. Upadhyay, E. Henestroza, T. W. Hall, B. L. Musico, M. Sanchez Barrueta, E. Huang and A. M. Alexander. Study for Alternative Cavity wall and Inductive Insert Material\xc2\xa0. Presented at *LDRD-MFR phase 2 oral prentation*, Los Almos, New Mexico, United States, 2021-06-23 - 2021-06-23. (LA-UR-21-25754)

Wiggins, B. W., C. G. Richards, M. Iliev and M. P. Hehlen. Compact-High Dynamic Range Composites for Space Applications. Presented at *TECH TALK*, Los Alamos, New Mexico, United States, 2021-08-09 - 2021-08-09. (LA-UR-21-30343)

Using Laser Synthetic Aperture Radar to Image a Low Earth Orbit Satellite

David Thompson
20210435ER

Project Description

We have developed a novel imaging concept that could potentially achieve centimeter-scale imaging resolution at extremely long range, far beyond current state-of-the-art. This concept uses a modified radar technique, but illuminating the target with a laser and measuring the round-trip time of laser photons instead of radar emissions. We have already tested the technique on the ground at ranges up to 10 kilometer (km), and demonstrated better spatial resolution than that of a conventional imaging radar. We propose to demonstrate this imaging technique on a space object for the first time by laser-illuminating a satellite in low earth orbit (at a range of 500-1000km) from the Air Force Research Laboratory's Starfire Optical Range (SOR) in Albuquerque, and detecting return photons on the ground (also at SOR), as the satellite angle changes during a pass overhead. The experiment will further develop the experimental technique and the required data analysis techniques. Future mission areas that could be enabled by this research include space treaty verification, planetary defense against earth colliding asteroids, and missile defense. This novel imaging approach has transformational impact, enabling new classes of long-range, high-resolution imaging missions for both national security and basic science.

Publications

Journal Articles

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. C. Thompson and D. Palmer. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Submitted to *Applied Optics*. (LA-UR-21-29582)

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. Palmer and D. C. Thompson. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Submitted to *Applied Optics*. (LA-UR-21-32462)

Presentation Slides

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. C. Thompson and D. Palmer. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Presented at *Imaging and Applied Optics Congress*, Vancouver, Canada, 2021-07-19 - 2021-07-23. (LA-UR-21-22050)

Hoffmann, M. P., N. Dallmann, B. E. Carlsten, M. P. Coblentz, D. C. Thompson and D. Palmer. Incoherent Range-Based Holography of Far-Distant Objects Using LIDAR. Presented at *OSA Imaging and Applied Optics Congress*, Vancouver, Canada, 2021-07-19 - 2021-07-23. (LA-UR-21-26408)

Thompson, D. C. and J. A. Cox. Los Alamos National Laboratory Intelligence and Space Research Division. . (LA-UR-22-22551)

A Low Power Electron Injector for Space Applications

Michael Holloway
20210443ER

Project Description

One threat that could cripple critical space infrastructure is high energy electrons from solar wind or high altitude nuclear explosions that become trapped in the Earth's radiation belts. These electrons can cause electrostatic buildup and discharge on satellites causing critical damage. Radiation belt remediation is an important area of research being conducted at Los Alamos National Lab. One promising approach to mitigate this threat is to generate electromagnetic waves using a modulated electron beam from an accelerator in orbit. The work of this project is critical technology development of an electron source that will be required to develop an orbital electron accelerator to meet future radiation belt remediation experiments and operational missions. The electron source design innovations in this work will reduce complexity, improve efficiency and mechanical robustness, and will be scalable to meet future mission needs.

Uranium hexafluoride enrichment verification using ultra-low field nuclear magnetic resonance

Per Magnelind
20210770ER

Project Description

As new, large capacity, Gas Enrichment Centrifuge Plants (GECPs) are brought online, the inspection effort by the International Atomic Energy Agency that safeguards these facilities is an increasing burden. Verifying uranium enrichment is a key objective for GCEP safeguards. Existing technologies have a variety of strengths and weaknesses. Measurements are technically very challenging and prone to spoofing in high background radiation or highly dynamic production environments with conventional methods. However, Nuclear Magnetic Resonance (NMR) has the potential to improve the performance of such measurements, as it is inherently not sensitive to radiation and allows accurate measurement inside non-magnetic metallic packaging such as pipes with enriched Uranium hexafluoride (UF_6) gas. NMR provides a unique multi-peak signature from enriched UF_6 (uranium-235), as it is the only long half-life Uranium-isotope with a non-zero spin property. However, conventional NMR is not fieldable and cannot detect usable signals through pipes or containers. The zero to ultra-low field (ZULF) regime, 0–500 Nanoteslas (nT), has the potential for a portable/fieldable NMR technique to measure uranium enrichment. The method is non-invasive, can measure inside non-magnetic metallic packaging, and does not rely on ionizing radiation. An improved non-destructive enrichment verification technology would benefit onsite inspections of nuclear facilities worldwide.

Fission-Acoustic Signature Discovery

Rollin Lakis
20210853ER

Project Description

The objective of this work is to lay the foundation for the first experiments to "listen" for the sound of an individual fission event. When successful, this new signature will open many possibilities for the characterization of fissile materials in condensed matter, to study the evolution of defects in condensed matter and to potentially image fission events under extreme conditions. The fission-acoustic measurement can, in addition, open opportunities detect and characterize high consequence objects, and to monitor actinide processes.

Rapid Bioremediation and Simultaneous Enrichment of Uranium by Common Green Algae

Laura Lilley
20210869ER

Project Description

Research in green algae is a cornerstone of Department of Energy (DOE) research initiatives; isotopic fractionation is a cornerstone in the National Nuclear Security Administration (NNSA) mission space. Based on the observation that green algae are capable of uranium uptake and isotopic fractionation, we are investigating the mechanisms through which this process is governed. This fundamental understanding will enable us to 1) manipulate the uptake (bioremediation) and fractionation (energy) in cultures of green algae, 2) evaluate and anticipate potential clandestine threats (forensics), and 3) investigate a new research avenue for biologically-mediated isotopic separations (separation science).

Imaging Neural Dynamics With Ultra-Low Field Magnetic Resonance Imaging (MRI)

Per Magnelind
20180058ER

Project Description

This project will provide a new neuroimaging capability that will aid in different aspects of increasing the knowledge about the most complex system we know – the human brain. An increased fundamental understanding of the brain would have important implications in the vast field of neuroscience (e.g. within National Institutes of Health – NIH), and could have importance for national security by enhancing human performance through methods such as transcranial electrical stimulation and magnetic stimulation, which are of interest to numerous Department of Defense (DoD) sponsors, such as the Defense Advanced Research Projects Agency (DARPA).

Technical Outcomes

This project resurrected an ultra-low field (ULF) magnetic resonance imaging (MRI) system. The team implemented and improved sample temperature stability to increase the relaxation time of the liquid in the phantom, and a stable current source for injecting currents through phantoms. Inverse step-response data for pre-emphasized gradients was acquired to enable improved ULF MRI, especially inside shielded rooms. The team performed numerous imaging experiments with the improved system.

Publications

Presentation Slides

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-17-29752)

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-19-31476)

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Ultra-low field MRI and Current Density Imaging. Presented at *SBMT2018*, Los Angeles, California, United States, 2018-04-13 - 2018-04-13. (LA-UR-18-23160)

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Current-density imaging and magnetic resonance-based electrical impedance tomography at ultra-low fields. Presented at *Biomag2018*, Philadelphia, Pennsylvania, United States, 2018-08-26 - 2018-08-30. (LA-UR-18-28117)

Posters

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Current-density imaging and magnetic resonance-based electrical impedance tomography at ultra-low fields. Presented at *Biomag2018*, Philadelphia, Pennsylvania, United States, 2018-08-26 - 2018-08-30. (LA-UR-18-28116)

Proton Radiography for Advanced Cancer Therapy

Michelle Espy
20180238ER

Project Description

More than two dozen proton therapy centers now operate in the United States, taking advantage of the centimeter precision while minimizing the radiation absorbed in nearby healthy tissue. Even more precise proton treatments could target tumors on the order of a millimeter, or to tumors close to sensitive tissues, if relativistic proton beams (~1 gigaelectronvolt (GeV)) were used. The future of proton beam therapy will be at high energy, with direct, positive impact in treating the most difficult cancers, including some otherwise deemed untreatable, and those in the most radiation-sensitive, pediatric patients. Fully exploiting the precision of the higher-energy protons will require imaging both the patient and the dose deposition in real-time, on location, to ensure radiation accurately targets the tumor during each treatment. Fortunately, the same relativistic protons used for treatment can also be used to image tumors in a patient, as well as track treatment delivery. We propose to use the Los Alamos Neutron Science Center (LANSCE) Proton Radiography Facility to demonstrate imaging of small tagged tumors in mice with sufficient resolution and low enough dose to guide precise relativistic proton beam therapy. This work could profoundly influence the future development of proton therapy worldwide.

Technical Outcomes

Proton radiography was developed from a dynamic imaging technique, best suited for imaging high explosive driven dense materials, to a tool that can aid in the guidance of proton therapy treatments. The sensitivity limits of contrast enhanced proton radiography were established. A new type of proton radiography, dark field proton radiography, demonstrated a two-fold increase in sensitivity. In simulation, the technique was scaled down in energy, to match the systems clinically available in the U.S.

Publications

Journal Articles

Freeman, M. S., E. F. Aulwes, M. A. Espy, J. F. Hunter, P. E. Magnelind, F. E. Merrill, F. R. Trouw and D. Tupa. Direct Proton Detection for Therapy Guidance and Treatment Planning. Submitted to *Medical Physics*. (LA-UR-18-30411)

*Freeman, M. S., J. C. Allison, E. F. Aulwes, B. A. Broder, M. G. Davis, M. Espy, P. E. Magnelind, F. G. Mariam, L. I. Martinez, J. J. Medina, W. Z. Meijer, F. E. Merrill, C. Morris, L. P. Neukirch, K. P. Prestridge, A. Saunders, T. Schurman, R. B. Sidebottom, A. M. Tainter, Z. Tang, F. R. Trouw, D. Tupa, J. L. Tybo and C. H. Wilde. Dark field proton radiography. 2020. *Applied Physics Letters*. **117** (14): 144103. (LA-UR-20-23116 DOI: 10.1063/5.0021044)

*Sidebottom, R. B., J. C. Allison, E. F. Aulwes, B. A. Broder, M. S. Freeman, P. E. Magnelind, F. G. Mariam, F. E. Merrill, L. P. Neukirch, T. Schurman, J. Sinnis, Z. Tang, D. Tupa, J. L. Tybo, C. H. Wilde and M. Espy. Contrast-enhanced proton radiographic sensitivity limits for tumor detection. 2021. *Journal of Medical Imaging*. **8** (5): 053501. (LA-UR-20-28481 DOI: 10.1117/1.JMI.8.5.053501)

Conference Papers

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. G. Mariam, F. E. Merrill, D. Tupa and C. H. Wilde. Proton Radiography for Relativistic Proton Beam Therapy. Presented at *SPIE Medical Imaging*. (Houston, Texas, United States, 2018-02-12 - 2018-02-16). (LA-UR-18-20428)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, F. E. Merrill, P. E. Magnelind, D. Tupa and M. A. Espy. Gold nanoparticles for tumor detection with proton radiography: optimizing sensitivity and determining detection limits. Presented at *SPIE Photonics West*. (Virtual, New Mexico, United States, 2021-03-06 - 2021-03-06). (LA-UR-21-20944)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill, D. Tupa and M. A. Espy. Assessment of proton radiographic sensitivity limits for gold nanoparticle tagged tumors using gold leaf phantoms. Presented at *SPIE Medical Imaging*. (Houston, Texas, United States, 2020-02-16 - 2020-02-16). (LA-UR-20-20414)

Reports

Sidebottom, R. B. Gold-leaf phantoms of Au-tagged tumors to assess proton radiography for image guided proton therapy. Unpublished report. (LA-UR-19-23315)

Presentation Slides

Broder, B. A. Simulating Contrast in LANSCE's pRad System via TOPAS. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-26128)

Broder, B. A. Summary: LANL 2020 Internship. . (LA-UR-20-27155)

Espy, M. A. How to look at a brain. Presented at *NogginFest*, portland, Oregon, United States, 2018-10-19 - 2018-10-20. (LA-UR-18-29895)

Freeman, M. S. Magnetic focused proton radiography and its implications for proton beam guidance, anatomical alignment and adaptive therapy. Presented at *Annual Rocky Mountain Chapter Meeting of the American Association of Physicists in Medicine*, Colorado Springs, Colorado, United States, 2018-06-09 - 2018-06-09. (LA-UR-18-24975)

Freeman, M. S. Instantaneous Full Field Proton Radiography For Image Guidance. Presented at *American Association of Physicists in Medicine*, Nashville, Tennessee, United States, 2018-07-29 - 2018-08-02. (LA-UR-18-25530)

Freeman, M. S. Proton Radiography for Treatment Planning and Guidance. Presented at *UNM Medical Physics Symposium*, Albuquerque, New Mexico, United States, 2018-11-16 - 2018-11-16. (LA-UR-19-20477)

Freeman, M. S. Flash Proton Radiography for the Clinic: Real-Time Adaptive Therapy and a Proton-Based Estimate of Water-Equivalent Thickness. . (LA-UR-19-23520)

Freeman, M. S. Proton Radiography for Dense Dynamic Systems: a Capabilities Overview. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-31068)

Freeman, M. S. Hyperpolarized 129Xe MRI: Visualizing Lung Anatomy and Function. . (LA-UR-19-31585)

Freeman, M. S. Spin Physics. . (LA-UR-20-26492)

Freeman, M. S. Hyperpolarized 129Xe MRI Visualizing Lung Anatomy and Function. . (LA-UR-20-29731)

Freeman, M. S., E. F. Aulwes, L. Dong, T. Li, P. E. Magnelind, F. E. Merrill, L. P. Neukirch, R. Selwyn, R. Serda, R. B. Sidebottom, Z. Tang, K. Teo, D. Tupa, C. H. Wilde and M. A. Espy. Scaling the Ultra-Fast LANL System to Medical Energies. Presented at *58th Annual Meeting of the Particle Therapy Co-Operative Group*, Manchester, United Kingdom, 2019-06-10 - 2019-06-10. (LA-UR-19-25360)

Freeman, M. S., E. F. Aulwes, L. Dong, T. Li, P. E. Magnelind, F. E. Merrill, R. Selwyn, R. Serda, R. B. Sidebottom, K. Teo, D. Tupa and M. A. Espy. Residual-Energy Lens Focused Proton Radiography at Clinical Energies. Presented at

Annual Meeting of the American Association of Physicists in Medicine, San Antonio, Texas, United States, 2019-07-14 - 2019-07-14. (LA-UR-19-26544)

Freeman, M. S., J. C. Allison, M. A. Espy, J. J. I. Goett, J. D. Lopez, P. E. Magnelind, F. G. Mariam, J. J. Medina, F. E. Merrill, C. Morris, L. P. Neukirch, A. Saunders, A. M. Tainter, Z. Tang, F. R. Trouw, D. Tupa, J. L. Tybo and C. H. Wilde. Instantaneous Full Field Proton Radiography for Image Guidance. Presented at *Annual Meeting of the American Association of Physicists in Medicine*, Nashville, Tennessee, United States, 2018-07-22 - 2018-07-22. (LA-UR-18-26984)

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. E. Merrill and D. Tupa. Proton Radiography and Therapy. . (LA-UR-18-22459)

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-19-31476)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill, D. Tupa and M. A. Espy. Gold nanoparticles for tumor detection with proton radiography: optimizing sensitivity and determining detection limits. Presented at *SPIE Photonics West BiOS*, Virual, New Mexico, United States, 2021-03-06 - 2021-03-11. (LA-UR-21-21067)

Posters

Aulwes, E. F., M. S. Freeman, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. A. Espy. Developing a Treatment Planning Method for High-Energy Proton Therapy. . (LA-UR-19-27480)

Broder, B. A. and M. S. Freeman. TOPAS Model for Simulating Proton Radiography. Presented at *Research Computing Expo and Symposium*, chicago, Illinois, United States, 2019-11-05 - 2019-11-05. (LA-UR-19-30818)

Freeman, M. S., E. F. Aulwes, P. E. Magnelind, F. E. Merrill, L. P. Neukirch, R. B. Sidebottom, Z. Tang, D. Tupa and C. H. Wilde. Water Equivalent Thickness from Instantaneous Proton Radiographic Transmission Measurements. Presented at *International Meeting of the Particle Therapy Co-Operative Group*, Manchester, United Kingdom, 2019-06-10 - 2019-06-10. (LA-UR-19-25169)

Freeman, M. S., J. C. Allison, E. F. Aulwes, M. A. Espy, P. E. Magnelind, F. G. Mariam, J. J. Medina, W. Z. Meijer, F. E. Merrill, L. P. Neukirch, T. Schurman, R. B. Sidebottom, Z. Tang, F. R. Trouw, D. Tupa and J. L. Tybo. Dark Field Proton Radiography: A Proof of Principle. Presented at *Annual Meeting of the American Association of Physicists in Medicine*, online, New Mexico, United States, 2020-07-12 - 2020-07-12. (LA-UR-20-26318)

Freeman, M. S., M. A. Espy, J. J. I. Goett, P. E. Magnelind, F. G. Mariam, F. E. Merrill, R. B. Sidebottom, F. R. Trouw, D. Tupa and C. H. Wilde. Lens-Refocused Proton Radiography for Proton Beam Guidance. Presented at *Annual Meeting 57 of the Proton Therapy Co-Operative Group*, Cincinnati, Ohio, United States, 2018-05-21 - 2018-05-26. (LA-UR-18-23884)

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. G. Mariam, F. E. Merrill, D. Tupa and C. H. Wilde. Proton Radiography for Relativistic Proton Beam Therapy. Presented at *SPIE Medical Imaging 2018*, Houston, Texas, United States, 2018-02-12 - 2018-02-16. (LA-UR-18-20846)

Sidebottom, R. B., D. Tupa, E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill and M. A. Espy. Gold-leaf phantoms of AuNP-tagged tumors to assess proton radiography for image-guided proton therapy. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27565)

Sidebottom, R. B., D. Tupa, E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill and M. A. Espy. Assessment of proton radiographic sensitivity limits for gold nanoparticle tagged tumors using gold leaf phantoms. Presented at *SPIE Medical Imaging*, Houston, Texas, United States, 2020-02-16 - 2020-02-16. (LA-UR-20-20412)

OrganiCam: A High-Sensitivity Radiation-Hardened Imaging Organic Detector For Space and Programmatic Applications

Roger Wiens
20180244ER

Project Description

This is a dual-purpose project with applications for outer solar system and for high-radiation areas on Earth such as nuclear reactor cores or an accident area such as Fukushima. We plan to build a time-resolved fluorescence camera and spectrometer (OrganiCam) that will be able to observe and distinguish organic and mineral (e.g., heavy-element) fluorescence. In tune with the NASA applications, we will study and develop plans for an instrument that can survive and operate in a highly radioactive environment. Robots like the "Little Sunfish" now exploring the insides of the Fukushima reactor show that instruments of this type can be highly beneficial in surveying damage in a nuclear contamination zone. Careful use of electronic and optical components are required for such an environment and so our project will focus significant effort for this capability.

Technical Outcomes

The OrganiCam prototype instrument (sensor head) was built and it works. The instrument uses flight spare parts from SuperCam for the intensifier, relay, and charged coupled device (CCD) section. It uses a completely new design for the camera and spectrometer sections, developed and fabricated during this project as proposed. The lenses for the camera are highly radiation tolerant. A patent was registered, a paper was submitted, and OrganiCam won an R&D 100 award.

Publications

Journal Articles

. W. R. C. *. R. A. *. G. K. *. N. R. T. *. P. C. *. S. B. *. O. L. *. A. S. *. V. S. *. C. S. M. *. M. A. K. *. A. T. E. *. Q. H. *. S. S. K. *. D. M. *. L. S. P. *. M. S. Gasda, P. J., P. J. Gasda, R. C. Wiens, K. Ganguly, R. T. Newell, S. M. Clegg, S. P. Love, A. Reyes-Newell, C. Peterson, B. Sandoval, L. Ott, S. Adikari, S. Voit, H. Quinn and M. Dale. OrganiCam: a lightweight time-resolved laser-induced luminescence imager and Raman spectrometer for planetary organic material characterization. 2021. *Applied Optics*. **60 (13): 3753. (LA-UR-21-20845 DOI: 10.1364/AO.421291)

Presentation Slides

Ganguly, K., P. J. Gasda, C. D. Gleasner, C. Mensah, S. H. Adikari, H. M. Quinn, A. C. Watkins, S. P. Love, A. Misra, T. Acosta-Mayda, S. K. Sarma and R. C. Wiens. Survival, Genetic Modification, and Time-Resolved Laser-Induced Fluorescence Analysis of Bacteria Exposed to High-Dose Radiation Simulating Europa's Surface. Presented at *Europa Workshop*, Houston, Texas, United States, 2018-10-09 - 2018-10-12. (LA-UR-18-29555)

Ganguly, K., R. C. Wiens, P. J. Gasda, R. T. Newell, A. L. Reyes-Newell, B. F. Sandoval, M. E. Dale, S. H. Adikari, C. D. Gleasner, S. J. Voit, C. Mensah, D. T. Seagraves, S. A. Wender, A. K. Misra, S. K. Sharma, H. M. Quinn, S. M. Clegg and S. Maurice. Benchmarking Organic Detection Limits with OrganiCam, for Remote Sensing from an Ocean World Lander or from a Mars Helicopter Mission. Presented at *AGU Fall Meeting 2020*, Zoom meeting, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29775)

Watkins, A. C. and H. M. Quinn. Evaluation of Electronic Performance in the Europa Environment. Presented at *20th Topical Meeting of the Radiation and Protection Shielding Division*, Santa Fe, New Mexico, United States, 2018-08-26 - 2018-08-26. (LA-UR-18-28218)

Posters

Wiens, R. C., P. J. Gasda, A. K. Misra, T. E. Acosta-Maeda, S. K. Sharma, H. M. Quinn, K. Ganguly, R. T. Newell, S. M. Clegg, S. Maurice, C. Virmontois, S. P. Love, A. E. Nelson, L. A. Ott and B. F. Sandoval. Organicam: A Lightweight Time-Resolved Fluorescence Imager and Raman Spectrometer for Organic Detection and Characterization. Presented at *LANL Engineering Week*, Los Alamos, NM, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21405)

Wiens, R. C., P. J. Gasda, A. Misra, T. Acosta-Maeda, S. Sharma, H. M. Quinn, K. Ganguly, S. P. Love, A. E. Nelson, R. T. Newell, S. M. Clegg, S. Maurice, C. Virmontois, L. A. Ott and B. F. Sandoval. Organicam: a lightweight time-resolved fluorescence imager and raman spectrometer for icy world organic detection and characterization. Presented at *50th*

LPSC, The Woodlands, Texas, United States, 2019-03-18 - 2019-03-22. (LA-UR-19-22356)

Wiens, R. C., P. J. Gasda, H. M. Quinn, K. Ganguly, R. T. Newell, S. M. Clegg, S. P. Love, L. A. Ott, B. F. Sandoval, S. Maurice, C. Virmontois, A. K. Misra, T. E. Acosta-Maeda and S. K. Sharma. Organicam: A Lightweight Time-Resolved Fluorescence Imager and Raman Spectrometer for Organic Detection and Characterization. Presented at *American Geophysical Union Fall Conference*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32186)

Boron and Ribose in Clay: a Precursor for Life on Earth and Mars?

Patrick Gasda
20190238ER

Project Description

On Earth, there is a close association between life and the presence of clay minerals and boron. Clays and borates, separately, have been invoked as possible components for the origin of life on Earth. Our goal is to understand the signatures of boron-bearing clays so that they may be identified on Mars by rovers. If these signatures are identified on Mars, they will address one of the highest priority goals of the planetary science community: clear evidence of past or present microbial life on Mars.

Technical Outcomes

The project successfully tested ribose-borate-clay reactions in analog early Mars and Earth environments. The project determined how much borate clays can adsorb, the peak of borate adsorption on Mars clays is at a higher pH compared to Earth clays, and borate-clays potentially stabilize ribose. The results constrain borate behavior in groundwater on Mars and support the possibility that borate-clays may have played a role in the origin of life on Earth and potentially Mars.

Publications

Presentation Slides

Legett, S. A. A Tale of Two Borons: Carboniferous-Permian Paleoceanography and Potential Origins of Life on Mars. . (LA-UR-21-23229)

Legett, S. A., C. M. Yeager, P. J. Gasda, M. A. Nellessen, L. Crossey, E. Peterson, N. L. Lanza, A. L. Reyes-Newell, D. M. Delapp, A. Labouriau, R. C. Wiens, S. M. Clegg and D. Das. Exploring potential origins of life on Earth and Mars by determining ribose stability in mixtures of borate-bearing clays. Presented at *Clay Minerals Society Annual Meeting*, Virtual, New Mexico, United States, 2020-10-19 - 2020-10-19. (LA-UR-20-28529)

Legett, S. A., C. M. Yeager, P. J. Gasda, M. Nellessen, L. Crossey, E. Peterson, N. L. Lanza, A. L. Reyes-Newell, D. M. Delapp, A. Labouriau, R. C. Wiens, S. M. Clegg and D. Das. Ribose Stability in Solutions with Borate and Borate-Bearing Clays: Implications for Origins of Life on Earth and Mars. Presented at *Lunar and Planetary Science Conference*, Online, New Mexico, United States, 2021-03-15 - 2021-03-19. (LA-UR-21-22277)

Nellessen, M. A., P. J. Gasda, L. Crossey, E. Peterson, N. L. Lanza, A. L. Reyes-Newell, D. M. Delapp, C. M. Yeager, A. Labouriau, R. C. Wiens, S. M. Clegg, S. A. Legett and D. Das. Boron Adsorption onto Martian Clay Mineral Analogs. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-26975)

Nellessen, M. A., P. J. Gasda, L. Crossey, E. Peterson, N. L. Lanza, A. L. Reyes-Newell, D. M. Delapp, C. M. Yeager, A. Labouriau, R. C. Wiens, S. M. Clegg, S. A. Legett and D. Das. Boron Adsorption onto Martian Clay Mineral Analogs. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27649)

Posters

Nellessen, M., L. Crossey, P. J. Gasda, E. Peterson, N. L. Lanza, C. M. Yeager, A. Labouriau, R. C. Wiens and S. M. Clegg. Boron Adsorption In Clay Minerals: Implications For Martian Groundwater Chemistry And Prebiotic Processes. Presented at *Los Alamos Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26618)

Other

Nellessen, M. A., P. J. Gasda and L. Crossey. Boron Adsorption In Clay Minerals: Borate speciation modeling. Audio/Visual. (LA-UR-20-25598)

Reduced-profile Current-sheet Array (CSA) Antenna with Simpler Drive and Better Antenna Efficiency

MD Zuboraj
20190268ER

Project Description

The best antenna architecture for satellites today (the current-sheet array, or CSA) is not well suited for cubesat applications because the current CSA architecture has been optimized for ultra-high bandwidths (i.e., up to 900%) but not for compact size or aperture efficiency. Future cubesat-based national security missions will likely only need ~ 20% bandwidths, which allow us to reoptimize the CSA architecture with improved efficiency and smaller size. The impact of this technology development will be higher bandwidth communications on cubesats with greater directivity.

Technical Outcomes

This project designed a phased array of maximum 95% efficiency with 23 decibels relative to isotopic (dBi) gain, with a profile as small as 144 centimeter^2, and weight as low as 1.1 pounds, meeting all the attributes to become an attractive CubeSat antenna.

Publications

Posters

A. Zuboraj, M. R. and B. E. Carlsten. Beam-Current Loss in Emittance-Dominated High-Frequency Tubes. Presented at *IEEE Pulsed Power and Plasma Science Conference*, Orlando, Florida, United States, 2019-06-23 - 2019-06-28. (LA-UR-19-25558)

Quantum Metrology with an Atom Superconducting Quantum Interference Device (SQUID)

Changhyun Ryu
20190334ER

Project Description

Inertial sensing is essential in many critical national security missions. Although global positioning system (GPS)-based navigation can be used in ideal situations, when GPS service is denied or unavailable, an independent, accurate, inertial sensor is needed. Quantum metrology with an atom superconducting quantum interference device (SQUID) can increase the sensitivity in rotation sensing dramatically by utilizing macroscopic entanglement between angular momentum states. The successful completion of this project will demonstrate a revolutionary increase in rotation sensitivity from macroscopic entanglement. This will make it possible to develop a portable inertial sensor with the highest sensitivity for critical national security missions. This research is relevant to Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions of national security science in developing novel sensing technologies.

Technical Outcomes

During this project, two important technical outcomes were obtained. First, the observation of quantum interference of currents with an atomtronic superconducting quantum interference device was analyzed and published. Second, a theoretical study of rotational symmetry-breaking quantum phase transition has been performed to find a novel rotation sensing scheme that is expected to exceed the current state of the art sensitivity

Publications

Journal Articles

*Ryu, C., E. C. Samson and M. G. Boshier. Quantum interference of currents in an atomtronic SQUID. 2020. *Nature Communications*. **11** (1): 3338. (LA-UR-20-25170 DOI: 10.1038/s41467-020-17185-6)

Presentation Slides

Ryu, C. Quantum Metrology with an Atom SQUID. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31465)

Novel, Fast Enhancements to Bragg Ptychography

Kevin Mertes
20190373ER

Project Description

The ability to rapidly produce non-destructive, three-dimensional (3D) images of crystalline nanostructures with nanometer resolution is directly relevant to our nation's national security. This research will provide a versatile tool that meets the needs of Department of Energy-Basic Energy Sciences, Weapons Science and Global Security Intelligence and Emerging Threats.

Technical Outcomes

Tools successfully developed by this effort include: Mathematical models describing the propagation of coherent x-rays scanned across and through a sample; high-performance software that iteratively reconstructs a sample's complex transmissivity, as well as the beam profile and phase; and a pre-processing pipeline for automatic handling, conversion, and filtering of raw experimental data and a hardware/software solution to mitigate the position errors. All of these tools have been successfully applied to real data from imaging experiments.

Publications

Journal Articles

*Pound, B. A., K. M. Mertes, A. V. Carr, M. H. Seaberg, M. S. Hunter, W. C. Ward, J. F. Hunter, C. M. Sweeney, C. M. Sewell, N. R. Weisse-Bernstein, J. K. S. Baldwin and R. L. Sandberg. Ptychography at the Linac Coherent Light Source in a parasitic geometry. 2020. *Journal of Applied Crystallography*. **53** (5): 1276-1282. (LA-UR-19-32687 DOI: 10.1107/S1600576720010778)

Posters

Burdet, N. G., A. V. Carr, J. M. Bowlan, K. M. Mertes, J. D. Nguyen, R. Tobey, X. Ding, S. Lin, C. S. Walker, B. A. Pound, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins , V. Zapf, C. Mazzoli and R. L. Sandberg. Towards spatially mapping domain dynamics in Antiferromagnetic materials with soft x-ray scattering at NSLS-II. Presented at *SLAC Users Meeting*, Standford, California, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-25092)

Viral Mosaic Biosensor

Jessica Kubicek-Sutherland
20190392ER

Project Description

Influenza is a rapidly evolving viral pathogen that infects up to 5 million people annually. The early diagnosis and treatment of influenza infections can greatly reduce mortality. However, the currently available rapid influenza tests are unreliable and leave many infections undiagnosed. There is an urgent need for a highly sensitive influenza diagnostic test to be used in point-of-care settings. We will combine theoretical mosaic sequence design and the biosensor technology capabilities developed at Los Alamos National Laboratory to develop a rapid ultra-sensitive influenza biosensor using computationally-derived novel sequence probes that encompass a wide variety of influenza viruses to detect not only presently circulating viruses but potentially also future pandemic strains that will evolve through mutations and rearrangement. The resulting novel, inexpensive and highly sensitive diagnostic tool will be easily expandable to other pathogens, with influenza serving as a proof-of-principle. This work directly supports the Laboratory's Science of Signatures Pillar in threat reduction, biosurveillance and global health security and the missions of the DOE Office of Science Biological and Environmental Research (BER), as well as DHHS (NIH and CDC) missions to prevent, detect, diagnose, confront and treat disease, and is related to missions of DHS, DOD, and other federal agencies.

Technical Outcomes

The project developed a novel computational approach called FEVER (Fast Evaluation of Viral Emerging Risks) to design detection probes with: 1) broad-coverage biosurveillance of an entire class of viruses, 2) accurate diagnosis of an outbreak strain, and 3) mutation typing to detect variants of public health importance. FEVER probes for influenza and COVID-19 were used to detect viral Ribonucleic Acid (RNA) in human saliva using the Los Alamos waveguide-based optical biosensor and flow cytometer platforms.

Publications

Journal Articles

Courtney, S. J., Z. R. Stromberg, A. Gutierrez, D. Jacobsen, L. R. Stromberg, K. D. Lenz, J. Theiler, B. T. Foley, J. Gans, K. Yusim and J. Z. Kubicek-Sutherland. Optical Biosensor Platforms Display Varying Sensitivity for the Direct Detection of Influenza RNA. 2021. *Biosensors*. **11** (10): 367. (LA-UR-21-28484 DOI: 10.3390/bios11100367)

*Courtney, S. J., Z. R. Stromberg and J. Z. Kubicek-Sutherland. Nucleic Acid-Based Sensing Techniques for Diagnostics and Surveillance of Influenza. 2021. *Biosensors*. **11** (2): 47. (LA-UR-20-22835 DOI: 10.3390/bios11020047)

Kubicek-Sutherland, J. Z., J. P. Theiler, B. T. Foley, A. L. Myers y Gutierrez, A. D. Hollander, J. D. Gans, A. Deshpande, E. Martinez-Finley, H. Mukundan, K. Yusim and Z. R. Stromberg. Fast evaluation of viral emerging risks (FEVER) pipeline for detection and mutation typing of SARS-CoV-2. Submitted to *PLOS Global Public Health*. (LA-UR-21-21165)

Presentation Slides

Courtney, S. J. High-coverage diagnostic tool for SARS-like and influenza viruses. Presented at *Virtual interview presentation for University of Rochester PhD Program in Immunology, Microbiology, and Virology.*, Los Alamos, New Mexico, United States, 2021-02-05 - 2021-02-05. (LA-UR-21-20999)

Kubicek-Sutherland, J. Z. and S. J. Courtney. Beacons and Biosensors: An Approach to Influenza Diagnostics. . (LA-UR-20-25710)

Kubicek-Sutherland, J. Z. and Z. R. Stromberg. Investment Mentor Slides. . (LA-UR-20-23582)

Stromberg, Z. R. Development of SARS-CoV-2 RT-PCR Assays. . (LA-UR-20-29361)

Stromberg, Z. R. Development of a Fast Evaluation of Viral Emerging Risks (FEVER) Pipeline for Improved Diagnostics. Presented at *28th International Biodetection Technologies*, Virtual, New Mexico, United States, 2021-06-18 - 2021-06-18. (LA-UR-21-25264)

Posters

Courtney, S. J., Z. R. Stromberg, J. P. Theiler, B. T. Foley, J. D. Gans, K. Yusim and J. Z. Kubicek-Sutherland. High-coverage

nucleic acid probes for distinguishing SARS-CoV-2 from influenza. Presented at *Virtual Biophysical Society Annual Meeting 2021*, Los Alamos, New Mexico, United States, 2021-02-22 - 2021-02-26. (LA-UR-21-20318)

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

Emulating Quantum Magnetism with Rydberg Atoms

Michael Martin
20190494ER

Project Description

The goal of this project to create a reconfigurable and tunable system for quantum emulation, based on dynamically-configurable arrays of individually-trapped ultracold rubidium atoms. The character, range and strength of the interaction between the atoms will be tuned by the geometry of the arrays, and by external laser parameters. This complete set of capabilities will be the first highly scalable, neutral atom-based platform for tackling a broad range of models in quantum magnetism. By exploring system behavior, such as spin correlations and ground states, we will improve understanding of important quantum many-body models. Further, we will study coherent quantum annealing as an approach to quantum optimization problems, which will inform ongoing research on the properties of commercially-available quantum devices, for which the exact role of entanglement and coherence is poorly understood. This work will impact basic understanding of materials, by elucidating the role of entanglement in material properties, such as the so-called quantum spin liquid ground state; information science/technology, by establishing a testbed for solving complex optimization problems through a process known as coherent quantum annealing; and advanced quantum sensing, where control over interactions yields robust quantum states for sensing beyond classical limits.

Technical Outcomes

The team targeted a test-bed for quantum emulation based on a challenging experiment involving single-atom control, an ultraviolet laser, and an ultra-high vacuum system compatible with these requirements. Presently, the team has all the major experimental components of this system in place, including the most demanding subsystems, enabling future work in emulation (emulation was not demonstrated before the project end).

Publications

Journal Articles

Martin, M. J., Y. Jau, J. Lee, A. Mitra, I. H. Deutsch and G. W. Biedermann. A Molmer-Sorensen Gate with Rydberg-dressed atoms. Submitted to *PRX Quantum*. (LA-UR-21-29499)

*Mitra, A., M. J. Martin, G. W. Biedermann, A. M. Marino, P. M. Poggi and I. H. Deutsch. Robust M\xc3\xb8lmer-S\xc3\xb8rensen gate for neutral atoms using rapid adiabatic Rydberg dressing. 2020. *Physical Review A*. **101** (3): 030301. (LA-UR-19-31221 DOI: 10.1103/PhysRevA.101.030301)

Schine, N., A. Young, W. Eckner, M. J. Martin and A. Kaufman. Long-lived Bell states in an array of optical clock qubits. Submitted to *Nature*. (LA-UR-21-29502)

Reports

Martin, M. J., M. C. Revelle and G. W. Biedermann. A platform for quantum information and large-scale entanglement with Rydberg atoms in programmable optical potentials. Unpublished report. (LA-UR-18-31881)

Presentation Slides

Martin, M. J. Emulating quantum magnetism with Rydberg atoms. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31519)

Martin, M. J. Emulating quantum magnetism with Rydberg atoms. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31484)

Martin, M. J. Neutral atom tools for quantum information science. Presented at *Meeting at Argonne Natl. Lab*, Lemont, Illinois, United States, 2019-03-25 - 2019-03-25. (LA-UR-19-22592)

Martin, M. J. Quantum information science with Rydberg atoms. . (LA-UR-20-29116)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *UNM CQuIC seminar*, Albuquerque, New Mexico, United States, 2021-02-04 - 2021-02-04. (LA-UR-21-20920)

Martin, M. J. Quantum information science with laser-dressed atoms. Presented at *LANL/TAMU Quantum Seminar Series*, College Station, Texas, United States, 2021-04-27 - 2021-04-27. (LA-UR-21-23972)

Martin, M. J. Quantum information science and sensing with ultracold neutral atoms. . (LA-UR-21-25997)

Martin, M. J. Quantum information science with laser-dressed atoms Q-SEnSE Convergence Seminar. Presented at *Q-SEnSE Convergence Seminar*, Boulder, Colorado, United States, 2021-12-14 - 2021-12-14. (LA-UR-21-32107)

Martin, M. J., C. Ryu and M. G. Boshier. Quantum technologies with ultracold atoms. Presented at *UC Quantum Information Science Research Workshop*, Berkeley, California, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24127)

Martin, M. J. and M. G. Boshier. Ultracold atom-based quantum technologies. Presented at *Emerging Technology Virtual Nonproliferation Seminar Series*, Lemont, Illinois, United States, 2022-03-22 - 2022-03-23. (LA-CP-22-20181)

de Melo, L. F. Past and Present Research in Atomic Physics. . (LA-UR-20-28126)

Mitra, A., S. T. Omanakuttan, M. J. Martin, G. W. Biedermann and I. H. Deutsch. Fundamental limits of neutral atom entanglement using Rydberg dressing. Presented at *52nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, College Park, Maryland, United States, 2021-05-31 - 2021-06-04. (LA-UR-21-25172)

Discovering the 3D Structure and Dynamics of the Sun-Interstellar Medium System on a Global Scale

Daniel Reisenfeld
20190498ER

Project Description

The primary goal of this project is to understand the structure and dynamics of the Sun's space environment (the heliosphere) and its ability to screen the Earth from damaging radiation that is ubiquitous in the interstellar medium. Notably, this radiation, particularly cosmic rays, has a strong solar cycle variation; it also represents the greatest risk to interplanetary travel by humans as well as one of the largest backgrounds in National Nuclear Security Administration-sponsored, Los Alamos-built space instruments that detect nuclear explosions around the globe. The project exploits data from the Los Alamos-led energetic neutral atom (ENA) imager on the National Aeronautics Space Administration Interstellar Boundary Explorer (IBEX) mission to "sound" the three-dimensional extent of the heliosphere by monitoring over time the response of the outer heliosphere (via ENA emission) to bursts of plasma originally ejected from the Sun. By imaging the outer heliospheric response over time, we can understand the plasma flows and thus the underlying physical processes that govern heliospheric dynamics over the solar cycle. This research builds leadership capabilities in space weather and informs the optimization of the ENA imager that Los Alamos will lead for NASA's upcoming IMAP mission.

Technical Outcomes

This project had two main outcomes: (1) The first-ever empirical 3D map of the interstellar boundary, a bubble-like region of space surrounding the Sun that defines the boundary between our solar system and the rest of the galaxy, and (2) the development of a new validated data set using raw data from the NASA Interstellar Boundary Explorer (IBEX) mission, which has tripled the amount of data available for scientific analysis of the outer heliosphere.

Publications

Journal Articles

Reisenfeld, D. B., H. O. I. Funsten, M. Bzowski, J. Heerikhuisen, P. Janzen, M. Kubiak, D. J. McComas, N. A. Schwadron, J. Sokol, A. Zimorino and E. Zirnstein. A Three-Dimensional 1 Map of the Heliosphere from IBEX. Submitted to *Astrophysical Journal. Supplement Series*. (LA-UR-21-23228)

*Reisenfeld, D. B., M. Bzowski, H. O. Funsten, P. H. Janzen, N. Karna, M. A. Kubiak, D. J. McComas, N. A. Schwadron and J. M. Sokol. The Influence of Polar Coronal Holes on the Polar ENA Flux Observed by IBEX. 2019. *Astrophysical Journal Letters*. **879** (1): 1. (LA-UR-19-22264 DOI: 10.3847/1538-4357/ab22c0)

Reports

Reisenfeld, D. B. Discovering the 3D Structure and Dynamics of the Sun-Interstellar Medium System on a Global Scale Los Alamos LDRD Report. Unpublished report. (LA-UR-21-29072)

Presentation Slides

Kim, K. H. Survey of Ion Properties in Jupiter's Plasma Sheet. Presented at *Juno MWG Team Meeting*, Los Alamos, New Mexico, United States, 2020-07-31 - 2020-07-31. (LA-UR-20-25669)

Reisenfeld, D. B. Sounding the Dimensions of the Heliosphere with IBEX. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-28330)

Posters

Reisenfeld, D. B., M. Bzowski, H. O. I. Funsten, J. Heerikhuisen, P. Janzen, M. A. Kubiak, D. J. McComas, N. A. Schwadron, J. Sokol and E. Zirnstein. Building a 3-D Map of the Heliosphere with IBEX. Presented at *2020 Fall Meeting of the American Geophysical Union*, San Francisco, California, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29579)

Reisenfeld, D. B., M. Bzowski, H. O. I. Funsten, P. H. Janzen, M. A. Kubiak, D. J. McComas, N. A. Schwadron and J. Sokol. Sounding The Dimensions of the Heliosphere Using the Time-Correlation Between IBEX ENA Observations and the Solar Wind Dynamic Pressure. Presented at

Rare Earth Fission Product Element Separations by High Speed Counter-Current Chromatography

Iain May
20200116ER

Project Description

The rare earths are a series of elements that have very similar chemical properties, rendering their separation and purification extremely challenging. The analysis of radioactive rare earth elements adds significantly to this challenge. Our goal to to apply novel separation technology to significantly improve our ability to produce chemically and radiochemically pure samples. The separation and purification of rare earth elements supports multiple nuclear security and energy security missions.

Technical Outcomes

Through the use of High Speed Counter Current Chromatography (HSCCC) the team has demonstrated the successful separation of rare earth elements of relevance to fission product analysis. The tune-ability, and reproducibility, of the separation is one of the most striking successes of the project.

Gossamer Radio Frequency (RF) Satellite Parabola Made by Additive Manufacturing

Jeremiah Rushton
20200180ER

Project Description

This project will enhance the capability of orbital space assets. Its novel way to make a large dish for a compact satellite communication will be greatly disruptive for small-to-medium sized space assets. It is much more compact than any current technology and when developed will allow more agile design, faster design and rapid deployment of space assets for Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions dovetailing with other agencies. The patent-pending concept is simple; assemble a dish in orbit from compact, lightweight components.

Technical Outcomes

Significant progress was made by the team toward realizing a gossamer parabolic reflector. Rapid iteration between structural and electromagnetic analysis yielded a fabricable tape design, which was hand-assembled onto a base. Results verified structural elasticity and handling in a gravity environment. Revealed modal bending was addressed by adding a perpendicular rib tape which will enable assembly tractor attachment and mobility. Radiofrequency (RF) modelling also influenced improved tapes which have been fabricated. Assembly tractor concepts were matured.

Multi-Int Signature Collection and Exploitation for Security

Dale Anderson
20210706ER

Project Description

Characterization of adversary behavior by considering both moving and stationary energy sources would give insight into several National Security problems. This type of analysis is currently performed by expert analysts, which limits the number of sources that can be assessed and the timeliness of the reporting. This project aims to demonstrate the mathematical integration of transient and continuous wave time series signatures to characterize moving sources/targets. We hypothesize that time-varying sensor signatures (TVS) can be combined with time-stable sensor signatures to characterize relevant activities—and groupings of activities. The project will develop a reference dataset and methods that can automate this process to free up the analyst for assessment of the scenario and provide actionable results to decision makers. This work will advance the science by collecting a new and relevant dataset, developing new signatures, and analyzing them in combination with more traditional ones for improved source discrimination.

Technical Outcomes

The work was successful in achieving its goals and objectives in demonstrating that a passive seismo-acoustic tracking system is viable and could provide a cost-effective option for target detection, identification and tracking of small airborne and large ground-based vehicles. Unexpectedly, the field campaign occurred on the same day as a local earthquake, and analyses show that relevant time-varying signatures can be readily discriminated from background events such as local earthquakes.

Publications

Reports

Webster, J. D., J. D. Carmichael, E. M. Casleton, E. S. Schultz-Fellenz, B. M. Crawford, D. E. Coats, A. D. Collins, M. O. Gard, E. J. Guiltinan, D. M. Milazzo, R. D. Pratt, E. Swanson, M. L. Begnaud and D. Anderson. Multi-INT Signature Collection and Exploitation for Security: Improving Discrimination, Analyses, and Passive Tracking Capabilities for Time- and Distance-Varying Signatures in the Seismoacoustic Regime. Unpublished report. (LA-UR-21-29742)

Presentation Slides

Begnaud, M. L. Collecting and Analyzing Time- and Distance-varying Signatures (TVS, DVS) Using the LANL LARSA and UAS Systems. . (LA-UR-21-29577)

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

Daniel Reisenfeld
20210713ER

Project Description

The primary goal of this project is to understand the structure and dynamics of the Sun's space environment (the heliosphere) and its ability to screen the Earth from damaging radiation that is ubiquitous in the interstellar medium. Notably, this radiation, particularly cosmic rays, represents the greatest risk to interplanetary travel by humans as well as one of the largest backgrounds in National Nuclear Security Administration (NNSA)-sponsored, Los Alamos-built space instruments that detect nuclear explosions around the globe. The project goal is to develop an advanced method to construct statistically robust sky maps of the sun-interstellar medium interaction region using observations made by the Los Alamos-led Interstellar Boundary Explorer (IBEX)-Hi energetic neutral atom (ENA) imager on National Aeronautics and Space Administration 's (NASA's) IBEX mission. Our methods go far beyond the map reconstruction processes currently applied by the IBEX Science Operations Center, opening up the possibility of new discovery science with the IBEX data set, ultimately leading to a better understanding of how the interstellar boundary shields us from the incoming flux of cosmic rays.

Technical Outcomes

The project successfully demonstrated a new technique for rendering energetic neutral atom (ENA) sky maps of the heliosheath. The new maps are higher resolution and are capable of revealing structures that are not presently resolvable in standard Interstellar Boundary Explorer (IBEX) Science Operations Center (ISOC) maps.

Publications

Reports

Reisenfeld, D. B. Toward Discovering the Structure and Dynamics of the Sun-Interstellar Medium System Los Alamos LDRD Report. Unpublished report. (LA-UR-21-29381)

Presentation Slides

Osthus, D. A., B. P. Weaver, D. B. Reisenfeld, P. Janzen and E. Zirnstein. Generalized Ridge Regression Update: A Modified Graph Laplacian Approach. . (LA-UR-21-27973)

First Nuclear Quadrupole Resonance Observations of an Insensitive High Explosive

Michael Malone
20210719ER

Project Description

This work will explore new chemical signatures of the explosive triaminotrinitrobenzene (TATB) that is used in our nuclear stockpile. TATB is an insensitive high explosive that will only detonate under conditions far beyond what will detonate other explosives. This makes TATB the safe choice for our warheads because it reduces the possibility of unintended nuclear detonation. While TATB has been used for decades, there are a number of questions regarding its manufacturing and aging. We intend to measure a new property of TATB that will help address these questions. The nuclear quadrupole resonance (NQR) signals from materials results from the interaction of certain nuclei with their local electrical and magnetic environment. It is an extremely sensitive tool that has been demonstrated on a large number of other explosives but has not yet been observed for TATB. The NQR signal appears under certain experimental conditions. Using a set of related measurements, we are confident that we know the conditions to trigger an NQR signal in TATB. We will use these funds to observe the NQR signal of TATB. Once it is observed we can pursue new projects in applying NQR analyses to the technical problems of TATB manufacturing and aging.

Technical Outcomes

The experimental instrument was successfully built and found to have the desired signal to noise ratio. A suitable sample of triaminotrinitrobenzene (TATB) was obtained. Numerical predictions of the expected signal frequencies were obtained and showed excellent agreement with existing complementary experimental data. However, due to unanticipated restrictions a new lab space was needed. This greatly delayed the search and only a twentieth of the search area was tested and no signals were confirmed.

Active Electromagnetic Cloaking for Enhanced Science of Signatures

Abul Azad
20210779ER

Project Description

The ability to minimize electromagnetic scattering from an object and make it undetectable to external observers, known as invisibility cloaking, has been a fascinating topic both for the scientific community and intriguing applications. However, it not possible to create cloaking using natural material. . The advent of metamaterials and the emergence of transformation optics have enabled one of the biggest triumphs of the century in optical science and made cloaking a reality. Most of the demonstrated electromagnetic cloaks are passive in nature. A passive cloak can hide an object but the hidden object cannot communicate with the external network, requiring an active control of the cloak. In this project, we propose proposed to investigate the possibility of an active cloak design operating at microwave frequencies (6-10 gigahertz). We will design, fabricate, and characterize a multi-layered metasurface that allows active tuning of its complex optical properties to enable required cloaking parameters. Our goal is to obtain a few-layer cloak design-platform that allows integration of electrically tunable components through theoretical modeling and numerical simulations.

Technical Outcomes

The team developed a generic analytical formula to obtain the required phase gradient to achieve cloaking condition, designed the basic building block through full-wave numerical simulations, and fabricated the designed metasurfaces using in-house capabilities. The numerical studies exhibit the desirable amplitude and phase dispersion and switching of the ground plane from a reflector to a transmissive surface, a key featured for the active cloak. The team designed the basic building block through full-wave numerical simulations.

Publications

Journal Articles

R. Dalvit, D. A. and W. J. de Melo Kort-Kamp. Space-Time Dynamical Casimir effect. Submitted to *Universe*. (LA-UR-21-24200)

Presentation Slides

Goldhaber-Gordon, Z., A. E. Cardin and A. K. Azad. Broadband Active Metamaterial Microwave Cloaking. . (LA-UR-21-27660)

Data-Driven Specification of Earth's Magnetic Field

Humberto Godinez Vazquez
20210958ER

Project Description

As our society is increasingly dependent on technologies in space, predicting space weather becomes ever more important. We have come to rely on technologies such as cellphones, Global Positioning System (GPS), the Internet, and other commercial and military assets. In order to protect these systems a high priority is to develop better understanding of the harmful conditions of space weather encountered in the near-Earth radiation environment, which are mostly dictated by the dynamics of energetic charged particles. To predict satellite spacecraft hazards caused by space weather we are developing models that accurately simulate space weather close to Earth. These models leverage available measurements to provide a better prediction of the space environment. The main objective of this project is to improve the specification and forecast of the particle distribution in the Earth's inner magnetosphere using data assimilation together with machine learning (ML) algorithms in our ring current-atmosphere interactions model with self-consistent magnetic and electric fields (RAM-SCBE). Our final deliverable will be a model that is fast to run and can accurately predict space weather events that is harmful to the nations satellite infrastructure.

Technical Outcomes

A series of "RAM-SCBE" model simulations were generated to fully describe the dynamics between the the electric fields and magnetic fields and the pressure field in the model. The generated solutions are being used to create a data-driven model that can provide the electric and/or magnetic field that takes as input the pressure field on the equatorial plane specified by RAM-SCBE. The methods employed are neural-networks, specifically a long-short term memory and a convoluted neural network.

Publications

Reports

Godinez Vazquez, H. C. Final Technical Report 20210958ER. Unpublished report. (LA-UR-21-32223)

Granddaughter Radiochronometry for Nuclear Forensics

Joanna Denton
20190565ECR

Project Description

To date there have been more than 2800 cases of nuclear material being found out of regulatory control. The illegal trafficking of such nuclear material poses a serious risk to global safety and security. Once nuclear material is interdicted, the discipline of nuclear forensics, alongside traditional forensics, attempts to identify a source, destination, and suspected use for the materials. The age, of a material, obtained through radiochronometry, is a key predictive signature in a nuclear forensics investigation. Currently, the age of a material can be obtained through parent-daughter radiochronometry. This project aims to add parent-granddaughter radiochronometry to the Laboratory's nuclear forensics toolbox enabling the age of a material to become more tightly constrained. Additionally, the results of this project will shed light on the behavior of uranium decay products during material processing and production. This information can be used as vital reference points for seizures of unknown uranium materials.

Publications

Presentation Slides

Denton, J. S., A. M. Wende, T. M. Kayzar-Boggs, M. A. Edwards and R. E. Steiner. Progress Towards a LANL Granddaughter Radiochronometry Capability. Presented at *BSAP Meeting*, Virtual, New Mexico, United States, 2021-02-09 - 2021-02-09. (LA-UR-21-20996)

Using Thundercloud Illumination by Lightning to Understand Optical Signal Propagation in Nature

Michael Peterson
20200529ECR

Project Description

Both nuclear explosions and natural phenomena (lightning, meteor impacts) produce bright flashes of light that can be detected from space. When optical signals have to travel through a cloud to reach the satellite, however, they can be modified by reflection / absorption interactions with raindrops and ice particles. These interactions cause optical space-based sensors like the National Oceanic and Atmospheric Administration's Geostationary Lightning Mapper (GLM) to miss lightning activity in large and dense clouds. They also leave a fingerprint on the optical signals that make it through to the satellite. The United States Department of Energy (DOE) supports development of optical and radio-frequency sensors for nuclear treaty monitoring. Those signals experience these same effects, so using lightning to better understand the propagation effects benefits sensor design and performance assessments in the United Stated Nuclear Detonation Detection System program.

Publications

Journal Articles

*Peterson, M. Holes in Optical Lightning Flashes: Identifying Poorly Transmissive Clouds in Lightning Imager Data. 2021. *Earth and Space Science*. **8** (2): e2020EA001294. (LA-UR-20-22888 DOI: 10.1029/2020EA001294)

*Peterson, M. Modeling the Transmission of Optical Lightning Signals Through Complex 3-D Cloud Scenes. 2020. *Journal of Geophysical Research: Atmospheres*. **125** (23): e2020JD033231. (LA-UR-20-23479 DOI: 10.1029/2020JD033231)

*M. D. *. B. D. Peterson, M. *. and M. Peterson. A Global LIS/OTD Climatology of Lightning Flash Extent Density. 2021. *Journal of Geophysical Research: Atmospheres*. **126** (8): e2020JD033885. (LA-UR-20-26320 DOI: 10.1029/2020JD033885)

*Peterson, M. J. Where are the Most Extraordinary Lightning Megaflashes in the Americas?. 2020. *Bulletin of the American Meteorological Society*. 1-26. (LA-UR-20-23234 DOI: 10.1175/BAMS-D-20-0178.1)

Peterson, M. J. The Illumination of Thunderclouds by Lightning: 1. The Extent and Altitude of Optical Lightning Sources. 2022. *Journal of Geophysical Research: Atmospheres*. **127** (1): e2021JD035579. (LA-UR-21-22307 DOI: 10.1029/2021JD035579)

Peterson, M. J. The Illumination of Thunderclouds by Lightning: Part 3: Retrieving Optical Source Altitude. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-21-23257)

Peterson, M. J. FORTE Measurements of Global Optical Lightning Waveforms and Implications for Optical Lightning Detection. Submitted to *Earth and Space Science*. (LA-UR-21-32433)

Peterson, M. J. Combined Optical and Radio-Frequency Perspectives on the Time Evolution of Lightning Measured by the FORTE Satellite. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-22-20047)

Peterson, M. J., T. E. Lavezzi Light and D. Mach. The Illumination of Thunderclouds by Lightning: Part 2: The Effect of GLM Instrument Threshold on Detection and Clustering. Submitted to *Earth and Space Science*. (LA-UR-21-22572)

Peterson, M. J., T. Lang, T. Logan, C. W. Kiong, M. Gijben, R. Holle, I. Kolmasova, M. Marisaldi, J. Montoya, S. D. Pawar, D. Zhang, M. Brunet and R. S. Cerveny. New WMO Certified Megaflash Lightning Extremes for Flash Distance (768 km) and Duration (17.01 seconds) Recorded from Space. 2022. *Bulletin of the American Meteorological Society*. (LA-UR-21-29056 DOI: 10.1175/BAMS-D-21-0254.1)

Peterson, M. J. and D. Mach. The Illumination of Thunderclouds by Lightning: 4. Volumetric Thunderstorm Imagery. Submitted to *Earth and Space Science*. (LA-UR-21-25408)

Peterson, M. J. and G. Stano. The Hazards Posed by Mesoscale Lightning Megaflashes. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-20-25866)

Presentation Slides

Mach, D., M. J. Peterson and M. Bateman. Current and Future Processing Techniques for Orbital Optical Lightning Sensors. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29634)

Peterson, M. J. Holes in Optical Lightning Flashes: Identifying Poorly-Transmissive Clouds in Lightning Imager Data. . (LA-UR-20-22698)

Peterson, M. J. Modeling Lightning Illuminating Complex 3D Cloud Scenes. . (LA-UR-20-23063)

Peterson, M. J. A CIERRA Gridded Product Climatology for LIS/OTD. . (LA-UR-20-24470)

Peterson, M. J. A New CIERRA Gridded Product Climatology for LIS/OTD. . (LA-UR-20-25628)

Peterson, M. J. GLM Observations of Extraordinary Lightning Including Two New World Lightning Records. Presented at *GLM Science Team Meeting*, Huntsville (Virutal), Alabama, United States, 2020-09-08 - 2020-09-10. (LA-UR-20-26389)

Peterson, M. J. Imaging Thunderclouds with the Geostationary Lightning Mapper. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29389)

Peterson, M. J. The Most Extraordinary Lightning Recorded by Satellites. Presented at *AMS Annual Meeting*, Online, New Mexico, United States, 2021-01-10 - 2021-01-15. (LA-UR-20-30220)

Peterson, M. J. and D. Mach. Documenting Lightning from Space with Optical and Radio-Frequency Sensors. Presented at *URSI_GASS*, Rome, Italy, 2021-08-28 - 2021-09-04. (LA-UR-21-27593)

Peterson, M. J. and D. Mach. Mapping Lightning in Three Dimensions with Optical Space-Based Lightning Imagers. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31100)

Peterson, M. J. and D. Mach. Volumetric Meteorological Imagery from the Geostationary Lightning Mapper. Presented at *102nd Annual Meeting of the American Meteorological Society*, Houston, Texas, United States, 2022-01-23 - 2022-01-27. (LA-UR-21-31446)

Posters

Peterson, M. J. Imaging Thunderclouds with the Lightning Imaging Sensor and Geostationary Lightning Mapper. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29572)

Stano, G. and M. J. Peterson. An Investigation of Geostationary Lightning Mapper Flash Extent. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29564)

Other

Peterson, M. J. GLM Full Disk Lighting Video. Audio/Visual. (LA-UR-20-23650)

Understanding Optical Signatures from Natural and Artificial Aurora

Rebecca Sandoval
20200555ECR

Project Description

Research using particle accelerators in space is critical to understanding how space weather affects the Earth, including negative effects on satellites and power grids. Space accelerators also have security applications, including reducing the impact of space radiation from a high-altitude nuclear explosion. Measuring accelerator performance in space, where laboratory instruments are not available, is a major challenge for developing the technology that enables these important missions. This project will develop a better way to measure accelerator performance by using an ultra-sensitive camera on the ground to capture the light produced when the beam from a space accelerator hits the atmosphere. First, we will develop measurement techniques by observing the natural aurora (Northern Lights), which produces a similar type of light. These tests will also capture the fastest video of the aurora ever recorded, which is expected to lead to important scientific discoveries about where the aurora originates. After developing experimental techniques by observing the aurora, we will actually measure the light from a space accelerator for the first time. By showing that we can assess how an accelerator performs from the ground, we will develop a valuable diagnostic tool for future science and security missions.

Publications

Presentation Slides

Sandoval, R. H. Space Research at Los Alamos National Laboratory. . (LA-UR-21-21850)

Other

Sandoval, R. H. and E. K. Emberton. Aurora photos for LDRD 20200555ECR. Audio/Visual. (LA-UR-21-24195)

Nitrogen: Abundant on Earth and Forgotten in Space

Philip Fernandes
20200580ECR

Project Description

Few measurements exist of nitrogen ions (N+) in the Earth's space environment, and most are from the 1970s–1990s. Modern literature treats N+ and O+ (oxygen ions) as interchangeable despite numerous measurements and models which show these ions behave very differently in space. Our poor knowledge of the differences in source, transport, and loss of N+ and O+ in the space environment hinders our ability to predict space weather, which is important for the Lab's space national security programs. Satellite measurements of O+ are used as a signature of geomagnetic storms: sun-driven disturbances that have broad, deleterious impact on the Nation, including radiation effects on satellites due to enhanced radiation belts, increased ionospheric scintillation that distorts radio, radar, and Global Positioning System (GPS) signals, and geomagnetically induced currents that can disrupt ground-based electrical power grids. Even more fundamental: our lack of knowledge of N+ transport prevents accurate understanding and prediction of the impact of a high-altitude nuclear explosion (HANE) on our space infrastructure, or detection of neighboring and potentially adversarial spacecraft (SDA: space domain awareness). We will develop a low-resource instrument capable of distinguishing N+ from O+, thus enabling addressing of mission-critical background measurements relevant to space weather, HANE, and SDA.

Publications

Journal Articles

Fernandes, P. A., G. L. Delzanno, M. H. Denton, M. G. Henderson, V. K. Jordanova, K. H. Kim, B. A. Larsen, C. A. Maldonado, E. G. D. Reeves, D. B. Reisenfeld and R. M. Skoug. Heavy Ions: Tracers and Drivers of Solar Wind/Ionosphere/Magnetosphere Coupling. Submitted to *Heliophysics 2050 white paper*. (LA-UR-20-27388)

Vira, A. D., B. A. Larsen, R. M. Skoug and P. A. Fernandes. Bayesian Model for HOPE Mass Spectrometers on Van Allen Probes. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-20-26079)

Posters

Fernandes, P. A., G. L. Delzanno, M. H. Denton, M. G. Henderson, V. K. Jordanova, K. H. Kim, B. A. Larsen, C. A. Maldonado, E. G. D. Reeves, D. B. Reisenfeld and R. M. Skoug. Heavy Ions: Tracers and Drivers of Solar Wind/Ionosphere/Magnetosphere Coupling. Presented at *Heliophysics 2050 Workshop*, Los ALamos, New Mexico, United States, 2021-05-03 - 2021-05-07. (LA-UR-21-25792)

A High-throughput (RapidPhage) Platform for the Discovery of Lytic Bacteriophages Against Multi-drug Resistance Pathogens

Anand Kumar
20210612ECR

Project Description

The universal decline in the effectiveness of antibiotics, combined with the dearth of newer antibiotics and the emergence of hard-to-treat bacterial pathogens, have driven the need to revisit alternatives to antibiotics. The use of bacteriophage therapy has shown assurance in addressing hard-to-treat bacterial pathogen infections but unfortunately, rapid discovery and isolation of novel phages remain significant challenges. The current gold standard technique to discover and isolate phages against specific pathogens relies on a classical plaque formation assay, which is low throughput, inefficient, and cumbersome. To overcome these limitations and advance the rapid discovery of therapeutic phages, we propose to develop a novel, widely applicable, high-throughput platform (named RapidPhage) to rapidly discover, isolate and characterize lytic phages against pathogens. As a proof of concept, we will apply the RapidPhage platform to discover methicillin-resistant Staphylococcus aureus (MRSA)-lytic phages. The outcome from this study will provide a novel, widely-applicable platform, which will substantially improve the discovery and isolation of lytic phages that are effective against the target pathogen of interest.

Locating Nature's Most Extreme Explosions in Real-time

Lucas Parker
20210675ECR

Project Description

CubeSats have been a disruptive force in the space industry, substantially reducing the cost and development time required to reach orbit, making it possible to rapidly deploy new space-based instruments. CubeSats and small satellites in general are now used for "agile space" national security missions. As an example, for monitoring applications a constellation of small satellites has clear advantages over that of a single large satellite. An obvious disadvantage of small satellites is their limited power budget, which in turn caps the computing capability of an instrument. How smart can a small satellite-borne instrument be if it only has a few watts of power allocated for computing? This project will pioneer the use of field programmable gate arrays (FPGAs) to perform the complex data analysis required for gamma-ray telescopes, achieving the high performance necessary for our analysis to be performed in real-time. FPGAs are a low-power computing resource, well suited for use on small satellites. This project targets an astrophysical application, but the employed techniques, including the use of artificial intelligence, can be applied to perform sophisticated edge computing on-board small satellites used for national security.

Publications

Journal Articles

Parker, L. P., S. Dahal, J. W. Appel, R. Datta, M. K. Brewer, A. Ali, C. L. Bennett, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. D. Couto, K. L. Denis, R. Dunner, J. Eimer, F. Espinoza, T. Essinger-Hileman, J. E. Colec, K. Harrington, K. Helson, J. Iuliano, J. Karakla, Y. Li, T. A. Marriage, J. McMahon, N. J. Miller, S. Novack, C. Nunez, K. Osumi, I. L. Padilla, G. Palma, M. A. Petroff, R. Reeves, G. Rhoades, K. Rostrem, D. A. N. Valle, D. J. Watts, J. L. Weiland, E. J. Wollack and Z. Xu. Four-year Cosmology Large Angular Scale Surveyor (CLASS) Observations: On-sky Performance at 40, 90, 150, and 220 GHz Frequency Bands. Submitted to *Astrophysical Journal*. (LA-UR-21-25008)

High Efficiency Active Environmental Sampling of Chemical Traces

Ann Junghans
20190517ECR

Project Description

The proposed work aims to deliver an active sampling matrix that enhances the Raman signature of a target analyte thereby enabling in-field analysis by handheld instruments. Successful completion of the proposed work could result in a disruptively new detection method for fast in-field analysis of traces of a multitude of Raman active chemicals (e.g. high explosives, hazardous chemicals, chemical and biological warfare agents) relevant for national security applications.

Technical Outcomes

The project combined use of polymeric gels, which are advantageous for sampling trace amounts of material in certain environments, and Surface Enhanced Raman Spectroscopy, which can lead to orders of magnitude higher signals of Raman active substances, such as high explosives or pharmaceuticals. The project was successful in increasing the signal of a previously not detectable surrogate material so that detection and identification with handheld instruments was possible, paving the way for fast in-field analysis.

Publications

Presentation Slides

Davis, E. S., S. A. Junghans, C. N. Hakoda and C. Pantea. Abstract for Acoustic manipulation of metallic particles for improved in-field material analysis Video. Presented at *180th Meeting of the Acoustical Society of America*, Online, New Mexico, United States, 2021-06-08 - 2021-06-10. (LA-UR-21-24468)

Davis, E. S., S. A. Junghans, C. N. Hakoda and C. Pantea. Acoustic manipulation of metallic particles for improved in-field material analysis. Presented at *180th Meeting of the Acoustical Society of America*, Online, New Mexico, United States, 2021-06-08 - 2021-06-10. (LA-UR-21-24596)

Posters

Junghans, S. A., S. Bajric, L. E. Wolfsberg, E. S. Davis, C. Pantea, G. S. Goff, B. L. Scott, R. E. Lakis and V. Henzl. High Efficiency Active Environmental Sampling of Chemical Traces. Presented at *LANL Global Security Symposium*, Los Alamos, New Mexico, United States, 2019-11-13 - 2019-11-13. (LA-UR-19-31344)

Understanding the Wave Mechanics of Micro-architected Waveguides to Design Acoustic Quick Response Codes

Vamshi Chillara
20190568ECR

Project Description

This project develops a first of its kind acoustic Quick Response (QR) code system that can store information in the acoustic wave response characteristics of structures. Acoustic QR codes do not broadcast information and cannot be tampered/intruded/compromised with any existing wireless technologies. Thus, they can provide an additional layer of security for applications in nuclear proliferation and global security. The outcomes of this research effort will have applications in chemical/biomaterials characterization and energy security.

Technical Outcomes

The project demonstrated a novel concept of using electromechanical resonances in piezoelectric wafers for information storage. The concept is referred to as a Piezoeelctric Quick Response (PQR) code and the stored information cannot be read using traditional techniques like optical scanning or radio waves. Thus, this technology offers enhanced security for applications in tagging and tracking. We demonstrated multi-bit PQR code that has significantly larger information storage capacity compared to what was originally proposed.

Publications

Journal Articles

*Chillara, V., C. N. Hakoda and C. Pantea. On the in-plane vibrations and electromechanical resonance characteristics of non-uniformly polarized rectangular piezoelectric wafers: selective mode-type excitation and specific mode enhancement. 2021. *Journal of Sound and Vibration*. 116129. (LA-UR-20-26559 DOI: 10.1016/j.jsv.2021.116129)

Chillara, V., J. J. Greenhall, C. N. Hakoda and C. Pantea. Electromechanical response of laterally clamped piezoelectric wafers: absence of in-plane mechanical resonances in the electromechanical impedance spectrum. Submitted to *Ultrasonics*. (LA-UR-20-30362)

Chillara, V., J. J. Greenhall and C. Pantea. Ultrasonic waves from radial mode excitation of a piezoelectric disc on the surface of an elastic solid. Submitted to *Ultrasonics*. (LA-UR-19-27754)

Guha, A., C. Pantea and V. Chillara. Tuning the relative strengths of electromechanical resonances using non-uniform polarization of piezoelectric wafers. Submitted to *IEEE Transactions on Ultrasonics, Ferroelectrics and Frequency Control*. (LA-UR-21-27837)

Hakoda, C. N., C. Pantea and V. Chillara. Multi-level frequency-specific information storage using engineered electromechanical resonances in piezoelectric wafer arrays. Submitted to *IEEE Transactions on Ultrasonics, Ferroelectrics and Frequency Control*. (LA-UR-21-27274)

Hakoda, C. N., E. S. Davis, C. Pantea and V. Chillara. Piezoelectric Quick Response (PQR) codes with multi-level information storage. Submitted to *Physical Review Applied*. (LA-UR-20-23220)

Hakoda, C., C. Pantea and V. K. Chillara. Engineering the beat phenomenon of quasi-Rayleigh waves for regions with minimal Surface Acoustic Wave (SAW) amplitude. 2021. *Journal of Sound and Vibration*. **515**: 116444. (LA-UR-21-23560 DOI: 10.1016/j.jsv.2021.116444)

*Hakoda, C., V. K. Chillara and C. Pantea. The effect of a transducer's spatial averaging on an elastodynamic guided wave's wavenumber spectrum. 2021. *Ultrasonics*. **114**: 106422. (LA-UR-20-25258 DOI: 10.1016/j.ultras.2021.106422)

Conference Papers

Hakoda, C. N., C. Pantea and V. Chillara. Investigation of resonance enhancement through non-uniform piezoelectric polarization for information storage methodology. Presented at *SPIE Smart Structures + NDE 2020 - New Digital Forum*. (Anaheim, California, United States, 2020-04-26 - 2020-04-30). (LA-UR-20-22867)

Presentation Slides

Chillara, V. Non-traditional information storage using acoustics and vibrations. . (LA-UR-20-27431)

Chillara, V. Engineering the electromechanical response of piezoelectric transducers. Presented at *180th meeting of the Acoustical Society of America*, Los Alamos, New Mexico, United States, 2021-06-08 - 2021-06-10. (LA-UR-21-24403)

Chillara, V. Ultrasonics for multiphase flow sensing and collimated beam imaging. . (LA-UR-22-22492)

Hakoda, C. N., C. Pantea and V. Chillara. Engineering the quasi-Rayleigh wave's beat phenomenon for embedded information storage. . (LA-UR-20-25201)

Hakoda, C. N., C. Pantea and V. Chillara. Wavelength-dependent radiator for improved non-contact measurements of elastodynamic guided waves. Presented at *180th Meeting of the ASA: Acoustics in Focus*, Los Alamos, New Mexico, United States, 2021-06-08 - 2021-06-10. (LA-UR-21-24105)

Hakoda, C. N., C. Pantea and V. Chillara. Wavelength-dependent radiator for improved non-contact measurements of elastodynamic guided waves. Presented at *The 180th Meeting of the Acoustical Society of America: Acoustics in Focus*, Online, New Mexico, United States, 2021-06-08 - 2021-06-10. (LA-UR-21-25407)

Hakoda, C. N. and V. Chillara. Backup Figures for ongoing publication. . (LA-UR-21-27001)

Posters

Hakoda, C. N., C. Pantea and V. Chillara. Investigation into form factors for mechanical-resonance-based methods of information storage. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21738)

Hakoda, C. N., C. Pantea and V. Chillara. Engineering the quasi-Rayleigh wave's beat phenomenon for embedded information storage. Presented at *IEEE International Ultrasonics Symposium*, Los Vegas, Nebraska, United States, 2020-09-06 - 2020-09-11. (LA-UR-20-26656)

In-Process, Full Part Defect Detection for Additive Manufacturing

Adam Wachtor
20190580ECR

Project Description

This work supports the national security mission by improving the capability to produce mission-critical parts through additive manufacturing. Additive manufacturing allows for the production of unique components without the need for significant preparation and tooling costs seen in traditional fabrication processes. These advances in non-destructive evaluation for in-process additive manufacturing may lead to active feedback and control of the additive manufacturing process and benefit quality control and part certification. This in turn will allow for the production of reliable components in-house that support stockpile life-extension programs and retrofits and provide low-cost handling and tooling fixtures for fabrication services.

Technical Outcomes

Three-dimensional ultrasonic diagnostic measurements of additively manufactured parts were performed unobtrusively during the manufacturing process and measured signal features were validated through X-ray computed tomography to defects (geometry, pores) induced by the manufacturing process. A machine learning framework for defect feature extraction of process monitoring measurements and defect prediction model were developed for spatially mapped time-series data. Deep learning techniques were applied to simulation data sets of ultrasonic wavefield images to predict defect regions.

Publications

Journal Articles

Cummings, I. T., E. M. Jacobson, E. B. Flynn, B. M. Patterson, B. K. Hunter and A. J. Wachtor. Detection of Lattice Defects in Additively Manufactured Metal Parts Using In-Situ Ultrasonic Inspection. Submitted to *Additive Manufacturing*. (LA-UR-22-22169)

Eckels, J. D., E. M. Jacobson, I. T. Cummings, I. F. Fernandez, K. Ho, N. Dervilis, E. B. Flynn and A. J. Wachtor. Predicting local material thickness from steady-state ultrasonic wavefield measurements using a convolutional neural network. 2022. *Ultrasonics*. 106661. (LA-UR-21-21310 DOI: 10.1016/j.ultras.2021.106661)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, N. Calta, G. Guss, J. Forien, M. Matthews and P. Depond. In-Situ Process Monitoring of Laser Sintering via Classification of Acoustic Emissions. Submitted to *Additive Manufacturing*. (LA-UR-20-26003)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, P. Depond, J. Forien, G. Guss, N. Calta and M. Matthews. Detection of Keyhole Pore Formation in Laser Powder-Bed Fusion Using Acoustic Process Monitoring Measurements. Submitted to *Additive Manufacturing*. (LA-UR-21-28830)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, P. Depond, J. Forien, G. Guss, N. Calta and M. Matthews. Sensor-Fusion of Pyrometry and Acoustic Measurements for Localized Keyhole Pore Identification in Laser Powder-Bed Fusion. Submitted to *Journal of Materials Processing Technology*. (LA-UR-22-20210)

Tempelman, J. R., M. K. Mudunuru, S. Karra, A. J. Wachtor, E. B. Flynn, B. Ahmmed, J. Forien, G. Guss, M. Matthews, P. Depond and N. Calta. Machine Learning to Discover Pore Formation Signatures and Predict Pore Location during Additive Manufacturing Process. Submitted to *Additive Manufacturing*. (LA-UR-20-26174)

Conference Papers

Cummings, I. T., E. M. Jacobson, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. IN-PROCESS DEFECT DETECTION FOR ADDITIVELY MANUFACTURED METAL LATTICES. Presented at *IMECE\xc2\xae International Mechanical Engineering Congress & Exposition*. (Portland, Oregon, United States, 2020-11-15 - 2020-11-19). (LA-UR-20-23494)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. Defect Detection in Additively Manufactured Metal Parts Using In-Situ Steady-State Ultrasonic Response Data. Presented at *International Mechanical Engineering Congress & Exposition*. (Portland, Oregon, United States, 2020-11-13 - 2020-11-18). (LA-UR-20-23495)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. DEFECT DETECTION IN ADDITIVELY MANUFACTURED METAL PARTS USING IN-SITU STEADY-

STATE ULTRASONIC RESPONSE DATA. Presented at *International Mechanical Engineering Congress & Exposition (IMECE)*. (Portland, Oregon, United States, 2020-11-13 - 2020-11-13). (LA-UR-20-25128)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. Using Steady-State Ultrasonic Direct-Part Measurements for Defect Detection in Additively Manufactured Metal Parts. Presented at *International Modal Analysis Conference (IMAC)*. (Virtual, New Mexico, United States, 2021-02-08 - 2021-02-11). (LA-UR-20-30178)

Presentation Slides

Cummings, I. T., E. M. Jacobson, A. J. Wachtor and E. B. Flynn. Acoustic Steady-State-Excitation Spatial Spectroscopy (ASSESS). Presented at *DisrupTECH Texas A&M Design Sprint Workshop*, Online, New Mexico, United States, 2021-02-24 - 2021-02-26. (LA-UR-21-21542)

Cummings, I. T., E. M. Jacobson, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. In-Process Defect Detection for Additively Manufactured Metal Lattices. Presented at *ASME International Mechanical Engineering Congress & Exposition 2020*, Online, New Mexico, United States, 2020-11-16 - 2020-11-19. (LA-UR-20-27464)

Jacobson, E. M., I. T. Cummings, E. B. Flynn and A. J. Wachtor. In-Situ Direct Inspection of Additively Manufactured Metal Parts. Presented at *Engineer's Week*, Los Alamos, New Mexico, United States, 2021-02-22 - 2021-02-25. (LA-UR-21-21603)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, A. J. Wachtor and E. B. Flynn. IMECE 2020 Video Presentation Script and Abstract. Presented at *ASME IMECE 2020*, Portland, Oregon, United States, 2020-11-16 - 2020-11-19. (LA-UR-20-27467)

Jacobson, E. M., I. T. Cummings, P. H. Fickenwirth, E. B. Flynn and A. J. Wachtor. IMAC XXXIX 10532: Using Steady-State Ultrasonic Direct-Part Measurements for Defect Detection in Metal Additively Manufactured Parts. Presented at *IMAC XXXIX*, Online, New Mexico, United States, 2021-02-08 - 2021-02-11. (LA-UR-20-30509)

Mellos, G. N., P. H. Fickenwirth, C. J. Montgomery, A. J. Wachtor and E. B. Flynn. Estimating Porosity of AM Constructed 304L SS Cylinders Using Process Parameters. . (LA-UR-19-26285)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, G. Guss, J. Forien, N. Calta and M. Matthews. In-Situ Process Monitoring for Defect Prediction in Laser Powder Bed Fusion. Presented at *Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-25. (LA-UR-20-21832)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, G. Guss, P. Depond, J. Forien, N. Calta and M. Matthews. Multi-Channel Process Monitoring of Laser Powder Bed Fusion. Presented at *ASTM International Conference on Additive Manufacturing*, Anaheim, California, United States, 2021-11-01 - 2021-11-05. (LA-UR-21-28966)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Feature Extraction of Acoustic Emissions. . (LA-UR-19-26291)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Sensor Fusion for Keyhole Identification in Laser Powder-bed Fusion Additive Manufacturing. Presented at *Los Alamos Student Symposium*, Los Alamos, New Mexico, United States, 2020-08-14 - 2020-08-14. (LA-UR-20-25464)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Updates on LANL AM Data Analysis. . (LA-UR-20-25768)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Acoustic Signal Processing for Online Defect Detection in Laser Powder-Bed Fusion. . (LA-UR-21-25772)

Wachtor, A. J. In-Process Quality Control of Additively Manufactured Parts. . (LA-UR-19-21711)

Wachtor, A. J., E. B. Flynn, E. M. Jacobson and I. T. Cummings. In-Situ Direct-Part Measurements for Defect Detection in Additively Manufactured Metal Parts. Presented at *2021 ASTM International Conference on Additive Manufacturing*, Anaheim, California, United States, 2021-11-01 - 2021-11-05. (LA-UR-21-30919)

Wachtor, A. J., J. R. Tempelman, E. B. Flynn, G. Guss, J. Forien, N. Calta and M. Matthews. In-Situ Acoustic Monitoring of Metal Powder Bed Fusion Processes. Presented at *Cross-JOWOG on AM*, Livermore, California, United States, 2020-01-27 - 2020-01-27. (LA-CP-20-20093)

Wachtor, A. J., J. R. Tempelman, E. B. Flynn, I. T. Cummings, E. M. Jacobson and B. M. Patterson. Defect Detection in Additively Manufactured Parts through In-Situ Monitoring and Direct-Part Inspection. Presented at *6th Cross-JOWOG Working Group Meeting on Applications, Design, and Certification of Additive Manufacturing*, Kansas City, Missouri, United States, 2022-02-28 - 2022-03-04. (LA-CP-22-20143)

Posters

Fickenwirth, P. H., C. J. Montgomery, E. B. Flynn and A. J. Wachtor. In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27760)

Jacobson, E. M., P. H. Fickenwirth, A. J. Wachtor and E. B. Flynn. Damage Detection in Metallic Additively Manufactured Parts using In-Situ Steady-State Ultrasonic Response Data. Presented at *LANL Engineer's Week 2020*, Los Alamos, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21545)

Mellos, G. N., P. H. Fickenwirth, C. J. Montgomery, E. B. Flynn and A. J. Wachtor. In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing. Presented at *LANL E-Week Poster Session*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-20. (LA-UR-19-21306)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. . (LA-UR-19-27835)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. . (LA-UR-19-27862)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. Presented at *Solid Free form Fabrication*, Austin, Texas, United States, 2019-08-12 - 2019-08-15. (LA-UR-19-28147)

New Innovations in Microtesla Nuclear Magnetic Resonance Spectroscopy

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20210679ECR

Project Description

The use of chemical warfare agents (CWAs) is a threat to national security and has been highlighted in the poisonings of Alexei Navalny and the Skripals. CWA use may occur domestically or on the battlefield. However, fieldable analysis of CWAs, vital for remediation and safety, remains an outstanding challenge. Recent developments in the field of microtesla Nuclear Magnetic Resonance (uT NMR) spectroscopy has identified unique spectral signatures, known as J-coupled spectrum (JCS), of nerve agent CWAs. However, the technology is limited by poor signal to noise ratios (SNR) and structure interpretations via JCS are virtually non-existent. This project will develop the necessary technologies to increase the signal, such that smaller quantities of nerve agent can be detected, and will develop structure-back prediction algorithms using machine learning. Thus, a JCS can now be acquired at lower (less lethal) concentrations and provide the likely structure, without prior knowledge. This is a significant advancement in the field of NMR spectroscopy and chemical sensing. Together, these results will make uT NMR the premier fieldable analytical tool for detection and identification of CWAs, with ties to the Department of Energy/National Nuclear Security Administration missions of non-nuclear forensics and chemical and biological weapon defense.

Technical Outcomes

The project was successful in developing a machine learning algorithm to identify molecular structure but was unsuccessful in deploying a hyperpolarization unit.

Publications

Journal Articles

Kaseman, D., M. Malone, A. Tondreau, M. A. Espy and R. F. Williams. Quantitation of Nuclear Magnetic Resonance Spectra at Earth's Magnetic Field. Submitted to *Journal of the American Chemical Society*. (LA-UR-21-26080)

Reports

Kaseman, D. Synopsis of Presentation "Detecting OP CWAs Using Low-Magnetic Field NMR Spectroscopy". Unpublished report. (LA-UR-21-25816)

Presentation Slides

Kaseman, D. Developments in Earth's Magnetic Field NMR for Industrial Applications. Presented at *PANIC*, Nashville, Tennessee, United States, 2021-10-17 - 2021-10-20. (LA-UR-21-29290)

Kaseman, D., R. F. Williams, M. A. Espy, J. L. Yoder, P. E. Magnelind, A. V. Urbaitis, M. T. Janicke, S. Widgeon Paisner, J. A. Mercer-Smith and L. M. Kisner. ERDE: Earth's-Field Resonance Detection and Evaluation Devices. . (LA-UR-21-23465)

Nelson, T. R. DFT for design and characterization of functional materials. . (LA-UR-21-22766)

Williams, R. F. and D. Kaseman. Forensic Detection of Chemical Warfare Agents Using Portable Low Magnetic Field Nuclear Magnetic Resonance – SEDONA and ERDE Devices. Presented at *32nd Session of the OPCW Scientific Advisory Board*, Virtual, New Mexico, United States, 2021-06-17 - 2021-06-17. (LA-UR-21-25508)

Improving Public Health by Linking Virus Genetic Evolution and Epidemic Spread

Arshan Nasir
20180751PRD3

Project Description

This project aims to develop models, methods, and applications based on the basic evolutionary biology of human viruses to better understand the epidemiology of human viral diseases and, ultimately to help intervene to reduce the burden of disease. Using public health data, including thousands of human immunodeficiency virus (HIV) sequences sampled from real populations, we will develop a computational framework to routinely retrieve virus sequence data (and associated metadata) from public health surveillance systems, apply standard and novel genetics and epidemiological models, and produce automated reports of HIV evolution and spread. This project ties in with the Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) National Security mission of forecasting and predicting biological threats. We focus specifically on the US HIV epidemic, working togheter with the Colorado and Michigan health departments, but our general framework will also be useful, with adaptations, in preventing other pathogen threats, such as Avian Flu, Ebola, Dengue, Zika and other rapidly evolving pathogens. Thus, this project strongly ties in with 'Pathogen Detection and Countermeasures' as well as 'Information Collection, Surveillance, and Reconnaissance' and 'Non-Nuclear Forensics' (as we will reconstruct the hidden who-infected-whom network).

Publications

Journal Articles

*Bokhari, R. H., N. Amirjan, H. Jeong, K. M. Kim, G. Caetano-Anollés and A. Nasir. Bacterial Origin and Reductive Evolution of the CPR Group. 2020. *Genome Biology and Evolution*. **12** (3): 103-121. (LA-UR-19-24949 DOI: 10.1093/gbe/evaa024)

*Hwang, K., H. Choe, A. Nasir and K. M. Kim. Complete genome of Polaromonas vacuolata KCTC 22033T isolated from beneath Antarctic Sea ice. 2021. *Marine Genomics*. **55**: 100790. (LA-UR-20-23340 DOI: 10.1016/j.margen.2020.100790)

*Mughal, F., F. Gul, A. Nasir and G. Caetano-Anolles. The origin and evolution of viruses inferred from fold family structure. 2020. *Archives of Virology*. **165** (10): 2177-2191. (LA-UR-20-23821 DOI: 10.1007/s00705-020-04724-1)

Nasir, A. Genetic Promiscuity in the Human Microbiome. Submitted to *Science*. (LA-UR-20-20701)

*Nasir, A., E. Romero-Severson and J. Claverie. Investigating the Concept and Origin of Viruses. 2020. *Trends in Microbiology*. **28** (12): 959-967. (LA-UR-20-24424 DOI: 10.1016/j.tim.2020.08.003)

Nasir, A., F. Mughal and G. Caetano-Anolles. The Tree of Life Describes a Tripartite Cellular World. Submitted to *Bioessays*. (LA-UR-20-30493)

*Nasir, A., G. Caetano-Anoll\xc3\xa9s and J. Claverie. Editorial: Viruses, Genetic Exchange, and the Tree of Life. 2019. *Frontiers in Microbiology*. **10**: 2782. (LA-UR-19-28355 DOI: 10.3389/fmicb.2019.02782)

Nasir, A., M. Dimitrijevic, E. Romero-Severson and T. K. Leitner. Large Evolutionary Rate Heterogeneity among and within HIV-1 Subtypes and CRFs. Submitted to *Genome Biology and Evolution*. (LA-UR-21-28214)

*Romero-Severson, E., A. Nasir and T. K. Leitner. What Should Health Departments Do with HIV Sequence Data?. 2020. *Viruses*. **12** (9): 1018. (LA-UR-20-25996 DOI: 10.3390/v12091018)

Books/Chapters

Nasir, A. and G. Caetano-Anolles. An early cellular origin of viruses. (LA-UR-19-24950)

Posters

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

Nasir, A., T. K. Leitner and E. Romero-Severson. Improving Public Health by Linking HIV Genetic Evolution and Epidemic Spread. Presented at *Sandia National Lab's Annual Postdoc Technical Showcase*, Albuqurque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-32531)

Disease Outcome Analysis for Improved Disease Interventions

Paul Fenimore
20190618PRD1

Project Description

This project addresses the need for radically improved multiplexing of both biothreat agent detection schemes and disease marker measurements (biothreat detection needs are exemplified by desired improvements to the Department of Homeland Security's Biowatch program). Improved instrumentation should address both problems. Quanlitatively better data is expected to lead to important advances in our analysis of multiple markers found in serious disease states and complex biothreat monitoring samples.

Smart Mobile Sensor Platform Development for Radiological Mapping of Large-Scale Areas

Tony Shin
20190625PRD2

Project Description

With the recent developments in drone technology and relatively low-cost radiation sensors (e.g., neutron and gamma-ray sensitive sensors) coupled with well-established statistical techniques, it is possible to implement an intelligent mobile sensor platform that exhibits an active learning methodology through continuous real-time observations of radiological signatures. We propose to develop a smart mobile sensor platform composed of several drones equipped with low-cost radiation sensors to develop a network of detectors that can efficiently survey and create high-fidelity radiological maps of large-scale areas. This work will demonstrate the potential benefits of utilizing technological advancements in drone technology and low-cost radiation sensors in conjunction with advanced active learning algorithms for radiological mapping of large-scale areas. It will demonstrate how the advanced active learning framework can be developed to ultimately improve on the speed and accuracy of the results. While this research will help improve on current radiological mapping capabilities, it will more generally explore how active learning algorithms can improve any decision making process, thus providing a versatile extension to other fields of interest.

Publications

Journal Articles

S. Shin, T. H., D. T. Wakeford and S. F. Nowicki. Multi-sensor optimal motion planning for radiological contamination surveys using prediction-difference maps. Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-20-26153)

Presentation Slides

S. Shin, T. H. Gaussian process regression for radiological contamination mapping. . (LA-UR-21-20338)

S. Shin, T. H. Gaussian process regression for radiological contamination mapping Applied to optimal motion planning for mobile sensor platforms. . (LA-UR-21-29400)

S. Shin, T. H. and S. F. Nowicki. Smart Mobile Sensor Platform Development for Radiological Mapping of Large-scale Areas. . (LA-UR-21-20339)

The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting

Christopher Johnson
20200681PRD1

Project Description

The national security challenge the project addresses is earthquake hazard from human-caused or natural earthquakes. The high-level goals of this research are to make dramatic advances in characterizing how earthquakes work during the entire earthquake cycle (from one earthquake to the next), and to attempt to dramatically advance earthquake forecasting—the time, location and magnitude of an earthquake. This work will develop the means to address earthquake hazard associated with energy extraction (geothermal, hydrocarbon) and waste storage (wastewater, carbon dioxide, nuclear). The work could also have significant impact to Ground Based Explosion Monitoring for developing approaches to identify anomalous sources. Although a high-risk research endeavor, the potential life-safety and economic impact of this proposal cannot be overstated. Moreover, this work will have broad impact to nearly all problems where prediction of brittle failure is crucial.

Publications

Journal Articles

Chen, K., T. Yeh, C. W. Johnson, C. Lin, Y. Lai and M. Shih. Whispering of the city: Characteristics and origin of environmental shaking in the Taipei metropolitan area. Submitted to *Geophysical Research Letters*. (LA-UR-21-20002)

Johnson, C. W., C. L. Hulbert, B. P. G. Rouet-Leduc and P. A. Johnson. Learning the low frequency earthquake daily intensity on the central San Andreas Fault. Submitted to *Geophysical Research Letters*. (LA-UR-20-28772)

Johnson, C. W., N. Lau and A. Borsa. An assessment of GPS velocity uncertainty in California. Submitted to *Earth and Space Science*. (LA-UR-20-29137)

*Meng, H., Y. Ben-Zion and C. W. Johnson. Analysis of Seismic Signals Generated by Vehicle Traffic with Application to Derivation of Subsurface Q-Values. 2021. *Seismological Research Letters*. **92** (4): 2354-2363. (LA-UR-20-26366 DOI: 10.1785/0220200457)

Xue, L., Y. Fu, C. W. Johnson, J. Otero-Tores, C. Shim and R. Burgmann. Seasonal seismicity in the Lake Biwa region of central Japan moderately modulated by lake water storage changes. Submitted to *Journal of Geophysical Research: Earth Surface*. (LA-UR-21-20003)

Reports

Johnson, C. W. and P. A. Johnson. The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting. Unpublished report. (LA-UR-21-25480)

Presentation Slides

Johnson, C. W. Probing fault systems using hydrospheric induced stress modulation. Presented at *GAGE/SAGE 2021 Community Science Workshop*, Online, NM, New Mexico, United States, 2021-08-17 - 2021-08-17. (LA-UR-21-26995)

Johnson, C. W., B. P. G. Rouet-Leduc and P. A. Johnson. Testing the ability of machine learning models to predict the timing of seismogenic nucleation. Presented at *AGU Fall Meeting 2020*, Online, NM, New Mexico, United States, 2020-12-07 - 2020-12-07. (LA-UR-20-29569)

Johnson, C. W. and P. A. Johnson. The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting. . (LA-UR-20-30323)

Johnson, C. W. and P. A. Johnson. The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting. . (LA-UR-21-20094)

Johnson, C. W. and P. A. Johnson. Microseismicity Deep Learning Model Developed and Applied to the Central U.S.. Presented at *AGU Fall Meeting 2021*, Online, NM, New Mexico, United States, 2021-12-13 - 2021-12-13. (LA-UR-21-31905)

Posters

Johnson, C. W. Identifying weak ground motions to characterize fault zone strain localization. Presented at *SCEC Rupture and Fault Zone Obervartory Workshop*,

Online, New Mexico, United States, 2021-04-13 -
2021-04-13. (LA-UR-21-23451)

The Next Generation of Aerosol Optical Models: Humidity Dependence and Chemical Processing

Manvendra Dubey
20200752PRD3

Project Description

Light absorbing particles from fires and explosions absorb sunlight reducing visibility and climate that can be enhanced if these particles take up water in humid air. The project will perform focused experiments to quantify these optical effects on targeted aerosols and analyze the results for predictive models. The results can be incorporated into atmospheric visibility, air quality, and climate models to improve forecasts for battlefield, wildfire, and climate impact response. It will also improve remote sensing for nuclear forensics and fire predictions on the battlefield. The results also have applications for next-generation photo-voltaic and nanomaterials for energy security.

Publications

Journal Articles

Gorkowski, K. J., C. Carrico and M. K. Dubey. Novel Molecular Framework Predicts Organic Aerosol Light Absorption. Submitted to *Nature Communications*. (LA-UR-21-32053)

*Sullivan, R. C., H. Boyer-Chelmo, K. Gorkowski and H. Beydoun. Aerosol Optical Tweezers Elucidate the Chemistry, Acidity, Phase Separations, and Morphology of Atmospheric Microdroplets. 2020. *Accounts of Chemical Research*. **53** (11): 2498-2509. (LA-UR-20-24435 DOI: 10.1021/acs.accounts.0c00407)

Reports

Gorkowski, K. J., S. H. Jordan, K. B. Benedict and M. K. Dubey. A novel approach to characterize the full spectrum and radiative properties of aerosols. Unpublished report. (LA-UR-21-28132)

Presentation Slides

Gorkowski, K. J., A. Rafferty, T. C. Preston, A. Zuend, R. Sullivan, N. Donahue, T. Capek, C. Mazzoleni, C. Carrico, J. E. Lee, A. C. Aiken and M. K. Dubey. One particle at a time: Insights from the Aerosol Optical Tweezers. Presented at *New Mexico Tech Seminar*, Los Alamos, New Mexico, United States, 2020-11-12 - 2020-11-12. (LA-UR-20-29250)

Gorkowski, K. J., A. Rafferty, T. Preston, A. Zuend, R. Sullivan, N. Donahue, T. Capek, C. Mazzoleni, C. Carrico, J. E. Lee, A. C. Aiken and M. K. Dubey. Exploring the outsized role humidity has on aerosol particles: Aerosol Optical Tweezers and Wildfires. Presented at *Georgia Technological University Invited Seminar*, Atlanta, Georgia, United States, 2020-09-24 - 2020-09-24. (LA-UR-20-27412)

Gorkowski, K. J., J. E. Lee, T. Capek, C. Mazzoleni, C. Carrico, A. C. Aiken and M. K. Dubey. Humidity Dependent Absorption Enhancements for Brown Carbon Surrogates. Presented at *American Association for Aerosol Research, Fall Meeting*, online, New Mexico, United States, 2020-10-05 - 2020-10-09. (LA-UR-20-27509)

Gorkowski, K. J., K. B. Benedict, J. E. Lee, A. C. Aiken, C. Carrico, T. Capek and M. K. Dubey. Humidity-Dependent Brown Carbon Light Absorption and Photobleaching: Laboratory and Model Synthesis of Organic Dyes.. Presented at *American Association for Aerosol Research 39th annual conference*, Albuquerque, New Mexico, United States, 2021-10-18 - 2021-10-22. (LA-UR-21-29966)

Gorkowski, K. J., K. B. Benedict, J. E. Lee, A. C. Aiken, C. Carrico and M. K. Dubey. Laboratory and Model Synthesis of Brown Carbon Dyes: Humidity-Dependence and Photobleaching. Presented at *Air and Waste Management Association: Atmospheric Optics: Aerosols, Visibility, and the Radiative Balance*, Bryce Canyon, Utah, United States, 2021-10-04 - 2021-10-08. (LA-UR-21-29546)

Gorkowski, K. J., M. K. Dubey, T. Capek, C. Carrico, K. B. Benedict, J. E. Lee and A. C. Aiken. Observing RH-Dependent Absorbing Aerosol Optics: Gray and Brown Carbon, and TRACER-CAT. Presented at *2021 ARM/ASR PI Meeting*, online, New Mexico, United States, 2021-06-21 - 2021-06-24. (LA-UR-21-25281)

Gorkowski, K. J., S. H. Jordan, K. B. Benedict and M. K. Dubey. A novel approach to characterize the complex refractive index spectrum of organic aerosols. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31762)

Gorkowski, K. J., S. H. Jordan and K. B. Benedict. A new approach to measure the light absorption of aerosols. . (LA-UR-21-27755)

Posters

Gorkowski, K. J., T. Capek, C. M. Carrico, J. E. Lee, A. C. Aiken, C. Mazzoleni and M. K. Dubey. Molecular Foundations of Humidity Dependent Absorption Enhancements by Brown Carbon Surrogates. Presented at *AGU Fall Meeting*, Online, New Mexico, United States, 2020-12-02 - 2020-12-02. (LA-UR-20-29463)

Superradiant RNA for Single Molecule In-Vivo Fluorescence Microscopy

Murray Wolinsky
20200774PRD4

Project Description

Understanding the genetic information encoded in deoxyribonucleic acid (DNA) has been increasing so rapidly that anyone can now sequence their genome and find potential markers for disease. However, we need a way to watch what our cells are doing in real time, where messages from the genome in the form of ribonucleic acid (RNA) are constantly changing. This project seeks to use aggregated groups of molecules assembled onto RNA as "addresses" for certain genes. These aggregates have optical properties that will allow them to be singled out in the complex environment of a cell. If successful, this project will produce a platform for establishing causal links between certain stimuli (e.g. pathogens, pharmaceuticals) and genetic responses, with the eventual goal of being able to predict a response on an individual level. This has wide-ranging implications for the development of medical treatments and response to biosecurity threats. For example, in the current coronavirus (COVID-19) pandemic, a small part of the population has a severe, fatal response to the virus, while the vast majority of the population has a mild response —we currently don't understand why this is, what if we could predict who will have a severe response and why ahead of time?

Publications

Journal Articles

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

Distinguishing Uranium Oxides using Table-top Extreme Ultraviolet Absorption Spectroscopy to Elucidate Reaction Kinetics and Conglomeration in Uranium-containing Laser Ablation Plasmas

Pamela Bowlan
20210916PRD2

Project Description

Forensics tools are needed for analyzing nuclear materials or debris. The commonly used visible and infrared spectroscopic tools have proven incapable of distinguishing different uranium oxides compounds. X-ray spectroscopy has proven to be a reliable approach for identifying uranium oxides, but typically requires taking these hazardous materials to synchrotrons. We propose instead to use a table top extreme ultraviolet (XUV) light source to provide the needed distinct signatures. Taking advantage of Los Alamos National Laboratory collaborators capabilities to grow high quality Uranium Oxide (U_xO_y) single crystal thin films, we will build a small library of the XUV signatures. As a next step, the same laser which we use to produce the XUV light will be used to create a uranium plasma, so that with the XUV spectroscopy, we can both produce and measure signatures of the U_xO_y conglomerates and also time-resolve their growth. This is highly relevant for mission relevant for developing novel signatures for nuclear forensics and for analyzing nuclear debris. The general concept to do work that is typically done at x-ray synchrotron at a table-top source at Los Alamos, has many potential mission relevant applications in forensics of other hazardous materials or materials in extreme conditions.

Publications

Presentation Slides

Skrodzki, P. J. Standoff laser-based optical spectroscopy of uranium enabled by ultrafast laser filamentation in air. . (LA-UR-21-28434)

How Biological Communities Can Unlock Hidden Signatures of Environmental Change

Jeanne Fair
20180715PRD2

Project Description

The Science of Signatures (SOS) pillar links the Laboratory's capability to pressing national needs in the Laboratory's primary mission areas of National Security Science, Global Security, and Emerging National Challenges. It does so by developing a scientific understanding of the origin and evolution of signatures and backgrounds, new measurement techniques and strategies for signature identification, and new analysis and interpretation tools for development of knowledge from these signatures. This project seeks to identify signatures of biological communities from the microbiome to forest communities in response to environmental change. Application of biological community signatures is relevant to global health security and threat reduction with pathogen detection as well as environmental change over time.

Technical Outcomes

Waiting for wildlife communities to decline following environmental change can take decades. After analyzing over 10 biological community datasets, this project found that wildlife microbiomes will be faster at detecting signatures of environmental change. The project's gained information will be used to improve experimental designs to further develop the use of microbiomes in detecting underlying threats to ecological systems. The project's results will help reduce threats to global health security by improving environmental change forecasting.

Publications

Journal Articles

*Abeyta, E. J., A. W. Bartlow, C. D. Hathcock and J. M. Fair. Individual Nest Site Preferences Do Not Explain Upslope Population Shifts of a Secondary Cavity-Nesting Species. 2021. *Animals*. **11** (8): 2457. (LA-UR-20-24957 DOI: 10.3390/ani11082457)

Ambrosiano, J. J., B. H. Sims, A. W. Bartlow, W. E. Rosenberger, M. R. Ressler and J. M. Fair. Ontology-Based Graphs of Research Communities: A Tool for Understanding Threat Reduction Networks. 2020. *Frontiers in Research Metrics and Analytics*. **5**. (LA-UR-19-31892 DOI: 10.3389/frma.2020.00003)

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

*Bartlow, A. W., C. Manore, C. Xu, K. A. Kaufeld, S. D. Valle, A. Ziemann, G. Fairchild and J. M. Fair. Forecasting Zoonotic Infectious Disease Response to Climate Change: Mosquito Vectors and a Changing Environment. 2019. *Veterinary Sciences*. **6** (2): 40. (LA-UR-19-22170 DOI: 10.3390/vetsci6020040)

Bartlow, A. W., M. Jankowski, C. D. Hathcock, R. Ryti, S. Reneau and J. M. Fair. Sex ratio of Western Bluebirds (Sialia mexicana) is mediated by phenology and clutch size. Submitted to *Ibis*. (LA-UR-21-23493)

Bartlow, A. W., Z. R. Stromberg, C. D. Gleasner, B. Hu, K. W. Davenport, S. Jakhar, P. Li, M. Vosburg, M. Garimella, P. S. G. Chain, T. H. Erkkila, J. M. Fair and H. Mukundan. Quantifying Intrinsic Bias in Diagnosis of Human Upper Respiratory Tract Infections – Implications for Early Diagnosis of Emerging Threats. Submitted to *Frontiers in Microbiology*. (LA-UR-20-25518)

Bartlow, A. W. and S. Bush. Faunal turnover of rodents following pi\xc3\xb1on-juniper expansion in the Great Basin. Submitted to *Biodiversity and Conservation*. (LA-UR-20-22841)

*Bartlow, A. W. and S. J. Agosta. Phoresy in animals: review and synthesis of a common but understudied mode of dispersal. 2021. *Biological Reviews*. **96** (1): 223-246. (LA-UR-19-22175 DOI: 10.1111/brv.12654)

Fair, J. M., J. Herman, C. D. Hathcock and A. W. Bartlow. A LONG-TERM STUDY OF THE EFFECTS OF BLOWFLIES ON THE GROWTH AND CONDITION OF SONGBIRD NESTLINGS. Submitted to *Oikos*. (LA-UR-20-24140)

*Musgrave, K., A. W. Bartlow and J. M. Fair. Long-term variation in environmental conditions influences host–parasite fitness. 2019. *Ecology and Evolution*. **9** (13): 7688-7703. (LA-UR-18-31593 DOI: 10.1002/ece3.5321)

Wysner, T. E., A. W. Bartlow, C. D. Hathcock and J. M. Fair. Long-term phenology of two North American secondary cavity-nesters in response to changing climate conditions. 2019. *The Science of Nature*. **106** (9-10): 54. (LA-UR-18-30750 DOI: 10.1007/s00114-019-1650-9)

Reports

Bartlow, A. W. How Biological Communities Unlock Signatures of Environmental Change. Unpublished report. (LA-UR-21-23624)

Presentation Slides

Bartlow, A. W. How biological communities can unlock hidden signatures of environmental change. . (LA-UR-20-30013)

Bartlow, A. W. Biosurveillance of zoonotic diseases to promote global health security. . (LA-UR-21-22579)

Fair, J. M. Bird communities and climate change. Presented at *Bird communities and climate change*, Los Alamos, New Mexico, United States, 2018-11-06 - 2018-11-07. (LA-UR-18-30737)

*Jacobs, L., B. H. McMahon, J. Berendzen, J. Longmire, C. Gleasner, N. W. Hengartner, M. Vuyisich, J. R. Cohn, M. Jenkins, A. W. Bartlow and J. M. Fair. California condor microbiomes: Bacterial variety and functional properties in captive-bred individuals. . (LA-UR-17-26676 DOI: 10.1371/journal.pone.0225858)

An Atomtronic Rotation Sensor

Malcolm Boshier
20180753PRD3

Project Description

This research will develop one approach to creating a so-called waveguide Sagnac atom interferometer. This device acts as an exquisitely sensitive rotation sensor. Rotation sensors are a key component of inertial navigation systems (INS). The atom interferometer sensor could potentially improve positioning accuracy with INS by an order of magnitude. Such an advance would be viewed as extremely important by agencies within DOD and the Intelligence Community (IC) who need precise positioning when Global Positioning System (GPS) is unavailable or denied. The device may also function as an accelerometer or gravimeter, which can be useful for detecting underground facilities relevant to non-proliferation and for finding mineral and oil deposits relevant to fossil fuels.

Technical Outcomes

The project developed a guided atom interferometer that used a collimated laser beam as a waveguide. The device can function an an accelerometer. The use of ultracold potassium atoms made non-interacting by the application of a suitable magnetic field increased the measurement time to almost one second, a factor of ten improvement in the state of the art. It also enabled 200 round-trips in the interferometer without significant degradation of the signal.

Publications

Journal Articles

Kim, H., K. A. Krzyzanowska, C. Ryu, K. C. Henderson, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple-loop atom interferometer. Submitted to *arXiv.org*. (LA-UR-20-28166)

Kim, H., K. A. Krzyzanowska, K. C. Henderson, C. Ryu, E. M. E. Timmermans and M. G. Boshier. One second interrogation time in a 200 round-trip waveguide atom interferometer. Submitted to *Physical Review Letters*. (LA-UR-22-20692)

Presentation Slides

Kim, H. Waveguide atom interferometer at LANL. . (LA-UR-21-22793)

Posters

Kim, H., J. Ferreras Fuertes, K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu and M. G. Boshier. Progress Toward Atomtronics Sagnac Interferometer. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28645)

Kim, H., K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu, E. M. E. Timmermans and M. G. Boshier. Demonstration of multiple round-trip waveguide atom interferometer. Presented at *APS DAMOP 2020*, Portland, Oregon, United States, 2020-06-01 - 2020-06-01. (LA-UR-20-23957)

Biophysical Interactions of Amphiphiles with Biomimetically Patterned Membranes

Loreen Stromberg
20190614PRD1

Project Description

Many of the biomarkers involved in infectious disease, cancer, and neurotraumatic conditions are lipids. The lipidic biochemistry is critical in determining the interaction of these biomarkers with membranes (which are also lipidic), blood, and other body fluids (which are aqueous). Yet, current methods for the measurement and detection of these biomarkers completely ignore their lipid biochemistry. Because of this, there is a significant failure rate in the adaptation of such technologies for real-world applications. Characterization, measurement, and understanding of these biomarkers in a physiological context can therefore revolutionize our ability to combat many conditions of relevance to human health. In this project, we will develop an ink-jet printing based method for the characterization and measurement of such lipidic biomarkers with membrane interactions, so as to enhance our understanding of human health without the need for animal models. This combines expertise in materials science, chemistry, modeling, and biological sciences and can provide new capabilities that can stretch beyond the biological sciences and influence materials science and environmental studies as well.

Technical Outcomes

The project worked on the development of strategies for the microscopic and spectroscopic characterization of lipid interactions with membranes. The team completed the work required to characterize the impact of complexity, as addressed by addition of components such as cholesterol and shingomyelin to lipid bilayers, on their ability to associate with other molecules, as well as on optimization of assays on a novel sensor platform for sensitivity and specificity.

Publications

Journal Articles

Courtney, S. J., Z. R. Stromberg, A. Gutierrez, D. Jacobsen, L. R. Stromberg, K. D. Lenz, J. Theiler, B. T. Foley, J. Gans, K. Yusim and J. Z. Kubicek-Sutherland. Optical Biosensor Platforms Display Varying Sensitivity for the Direct Detection of Influenza RNA. 2021. *Biosensors*. **11** (10): 367. (LA-UR-21-28484 DOI: 10.3390/bios11100367)

Stromberg, L. R., A. A. Bitzer, S. J. Courtney, S. Jakhar, K. E. Klosterman, J. Z. Kubicek-Sutherland, K. D. Lenz, L. M. Lilley, S. C. Moore, Z. R. Stromberg and H. Mukundan. Amphiphilicity in Host Pathogen Interactions – Implications for Bacterial Diagnostics. Submitted to *Microbiology and Molecular Biology Reviews*. (LA-UR-21-25880)

Presentation Slides

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

Posters

Stromberg, L. R., J. H. Werner, G. A. Montano and H. Mukundan. LPS-induced bilayer deformation is modulated with increasing lipid membrane complexity. Presented at *2019 CINT User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29418)

Stromberg, L. R., J. H. Werner, G. A. Montano and H. Mukundan. LPS-Induced Bilayer Deformation is Modulated with Increasing Lipid Membrane Complexity. Presented at *Biophysical Society Meeting*, San Diego, California, United States, 2020-02-15 - 2020-02-19. (LA-UR-20-21298)

Other

Stromberg, L. R., L. M. Lilley, M. Rush, K. D. Rector, G. A. Montano and H. Mukundan. Mechanisms of LPS-induced Lipid Bilayer Hole Formation (Imaging and Spectroscopy Dataset). Dataset. (LA-UR-21-25946)

Development and Implementation of a Portable Microfluidic J-Coupled Spectrometer for Rapid Detection and Identification of Emerging Chemical Threats

Derrick Kaseman
20190641PRD3

Project Description

This project will invent and develop new approaches for the detection of chemical warfare agents, chemical threat agents, pesticides, and insecticides. The detector is designed as a portable system that can be implemented domestically and internationally to help combat terrorism. The overarching goal of this project is to optimize a portable, fieldable detector that only uses earth's very small magnetic field to detect and identify minute quantities of chemical threats. This will be accomplished by optimizing a microfluidics-based spectrometer with a new detection system that reduces, by 10-fold, the total volume of sample required and the amount of sample in the volume by 1000-fold. This project ties into other Department of Energy national security missions by developing a unique technique for signature based, portable chemical sensing, which has important applications for military defense and homeland security.

Technical Outcomes

The project accomplished the goal of reducing the system volume and increasing the sensitivity by designing hardware improvements for the spectrometer that included increasing the prepolarizing magnetic field from 0.8 transmittance (T) to 1.93T by building a new Halbach magnet array. The system was further improved by integrating a 20 coil shim set into the system which increased the magnetic field homogeneity. Finally reducing the tubing diameter reduced the total system volume.

Publications

Journal Articles

*Kaseman, D. C., M. T. Janicke, R. K. Frankle, T. Nelson, G. Angles-Tamayo, R. J. Batrice, P. E. Magnelind, M. A. Espy and R. F. Williams. Chemical Analysis of Fluorobenzenes via Multinuclear Detection in the Strong Heteronuclear J-Coupling Regime. 2020. *Applied Sciences*. **10** (11): 3836. (LA-UR-19-30126 DOI: 10.3390/app10113836)

Kaseman, D., M. Malone, A. Tondreau, M. A. Espy and R. F. Williams. Quantitation of Nuclear Magnetic Resonance Spectra at Earth's Magnetic Field. Submitted to *Journal of the American Chemical Society*. (LA-UR-21-26080)

Kaseman, D., R. J. Batrice and R. F. Williams. Detection of Natural Abundance 13C J-couplings at Earth's Magnetic Field for Spin System Differentiation of Small Organic Molecules. Submitted to *Journal of the American Chemical Society*. (LA-UR-22-22496)

*Kaseman, D. and S. Sen. A review of the application of 2D isotropic-anisotropic correlation NMR spectroscopy in structural studies of chalcogenide glasses. 2020. *Journal of Non-Crystalline Solids*. 120500. (LA-UR-20-26008 DOI: 10.1016/j.jnoncrysol.2020.120500)

Reports

Kaseman, D. Synopsis of Presentation "Detecting OP CWAs Using Low-Magnetic Field NMR Spectroscopy". Unpublished report. (LA-UR-21-25816)

Presentation Slides

Kaseman, D. Nuclear Magnetic Resonance of Complex Material Systems: From Glasses to Chemical Warfare Agents. . (LA-UR-19-31588)

Kaseman, D. Chemical Warfare Agents Detection via Portable Low-Field Nuclear Magnetic Resonance. Presented at *Techwatch*, Washington D.C., Virginia, United States, 2020-03-11 - 2020-03-11. (LA-UR-20-22174)

Kaseman, D. Chemical Analysis of Small Molecules via NMR at Earth's Magnetic Field. Presented at *ACS Fall 2020*, San Francisco, California, United States, 2020-08-17 - 2020-08-17. (LA-UR-20-25767)

Kaseman, D. Earth's Field NMR for Detection of Chemical Warfare Agents. . (LA-UR-20-28887)

Kaseman, D. New Frontiers in Earth's Field NMR for Structure Elucidation. Presented at *NMR**2*, Virtual, New Mexico, United States, 2020-11-13 - 2020-11-13. (LA-UR-20-28961)

Kaseman, D. Developments in Earth's Magnetic Field NMR for Industrial Applications. Presented at *PANIC*, Nashville, Tennessee, United States, 2021-10-17 - 2021-10-20. (LA-UR-21-29290)

Kaseman, D., R. F. Williams, M. A. Espy, J. L. Yoder, P. E. Magnelind, A. V. Urbaitis, M. T. Janicke, S. Widgeon Paisner, J. A. Mercer-Smith and L. M. Kisner. ERDE: Earth's-Field Resonance Detection and Evaluation Devices. . (LA-UR-21-23465)

Williams, R. F. and D. Kaseman. Forensic Detection of Chemical Warfare Agents Using Portable Low Magnetic Field Nuclear Magnetic Resonance – SEDONA and ERDE Devices. Presented at *32nd Session of the OPCW Scientific Advisory Board*, Virtual, New Mexico, United States, 2021-06-17 - 2021-06-17. (LA-UR-21-25508)

Posters

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. New Frontiers in Nuclear Magnetic Resonance using Earth's Magnetic Field. . (LA-UR-19-28901)

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Identification of organophosphorus chemical warfare agents (CWAs), precursors, and decomposition products with a fieldable spectrometer using earth's magnetic field. Presented at *ACS Fall 2020*, San Francisco, California, United States, 2020-08-17 - 2020-08-17. (LA-UR-20-25766)

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Portable Earth's Field NMR Systems for the Detection of Chemical Warfare Agents. Presented at *PANIC*, La Jolla, California, United States, 2020-10-19 - 2020-10-22. (LA-UR-20-27477)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. A Fieldable Spectrometer Using Earth's Magnetic Field for Detection of Organophosphorus Nerve Agents. Presented at *Chemical and Biological Defense Science & Technology*, Cincinatti, Ohio, United States, 2019-11-17 - 2019-11-21. (LA-UR-19-31201)

Unraveling Lipoprotein Signatures for Tick-Borne Pathogens

Harshini Mukundan
20190655PRD4

Project Description

Vector borne pathogens present with different immunological signatures in the vector vs. the human host. These signatures are often the key towards unraveling their mode of action - be it immune evasion or activation- and lipidic molecules produced by the pathogen have a critical role to play in this response. In this project, we will use novel sensor technology together with lipoprotein measurement strategies in order to identify and unmask these critical signatures of Borrelia surface proteins, the causative agent of Lyme disease, in order to develop methods for rapid diagnostics and treatment of the infection.

Technical Outcomes

Lipidated signatures and their association with host lipoproteins have not been addressed in vector borne infections such as Lyme disease. The project aimed to explore lipidated signatures in tick-borne pathogens, and identified several signatures of relevance in Borrelia infection, although clinical and in vivo validation remains to be addressed in future studies. The project identified and evaluated the interactions of seven such lipoproteins during this post doctoral effort.

Publications

Journal Articles

Jakhar, S., A. A. Bitzer, L. R. Stromberg and H. Mukundan. Pediatric Tuberculosis: The Impact of "Omics" on Diagnostics Development. Submitted to *International Journal of Molecular Sciences*. (LA-UR-20-25709)

Stromberg, L. R., A. A. Bitzer, S. J. Courtney, S. Jakhar, K. E. Klosterman, J. Z. Kubicek-Sutherland, K. D. Lenz, L. M. Lilley, S. C. Moore, Z. R. Stromberg and H. Mukundan. Amphiphilicity in Host Pathogen Interactions – Implications for Bacterial Diagnostics. Submitted to *Microbiology and Molecular Biology Reviews*. (LA-UR-21-25880)

Neutron Spectroscopy for Nuclear Emergency Response Applications

Theresa Cutler
20210548MFR

Project Description

The nuclear emergency response mission may require disablement of a nuclear explosive device constructed and placed by an adversary. In order to render the device inoperable, its design must be understood. A combination of passive radiation signatures is used to reverse-engineer the design. Some plausible designs with complex neutron source terms have significant degeneracies in solution space, making absolute determination difficult and untimely. Neutron spectroscopy makes use of a passive signature that is rich with valuable information; however, no tool currently available makes use of this signature. We seek to develop such a tool and determine whether it can be a valuable addition to the toolkit. Our early work shows considerable promise. In Phase 1 we demonstrated the basic physics, interpretation of the raw signal, and signature penetrability through shielding. In Phase 2 we will optimize and ruggedize the system, including replacement of the liquid detector material with a more stable alternative, and we will test against realistic threat designs constructed in a Category-1 nuclear facility in Nevada.

Publications

Reports

Borgwardt, T. C., T. E. Cutler, K. Smith, K. D. Bartlett, C. R. Bates, K. C. Meierbachtol, D. J. Mercer, T. H. S. Shin and R. A. J. Weldon. Neutron Spectroscopy for NER Applications. Unpublished report. (LA-CP-21-20632)

Posters

Cutler, T. E., T. C. Borgwardt and K. Smith. Neutron Spectroscopy for NER Applications. . (LA-UR-21-25477)

Modeling an Artificial Radiation Belt of Ionized Fission Fragments After a High-altitude Nuclear Explosion (HANE)

Misa Cowee
20190528MFR

Project Description

The "Starfish mystery" refers to the unexpectedly widespread artificial radiation belt of beta-decay electrons created by the 1962 Starfish Prime High Altitude Nuclear Explosion (HANE) test shot, which fatally degraded ~1/3 of the satellites in orbit at the time. This widespread belt seemingly defied the laws of physics, as the ionized fission fragments which produced the beta-decay electrons should have been confined by magnetic fields, rather than transported far across them. A credible physical explanation of this effect has eluded the community for the last 50+ years, and is not included in current artificial radiation belt models. This lack of understanding is a limiting factor in our ability to accurately predict and prepare for this threat to satellites. In this project, we will develop a first-ever model to better understanding the motion and transport of ionized fission fragments on the seconds to hours timescales relevant to the formation of the belt taking into account several important loss processes. We will also better understand the threat posed to under-shielded satellites components, such as solar panels, from the ionized fission fragments themselves. Such knowledge is important to DOE/NNSA for predicting the man-made space environment and satellite hardening standards.

Technical Outcomes

The project successfully developed the proposed model capability and showed that high-altitude nuclear event/explosion (HANE) ionized fission fragments may form an artificial belt that persists in orbit for days until eroded by charge exchange with the atmosphere. For the scenario simulated, they posed a hazard to satellites only for certain situations where the solar cells have gaps in their protective coating. This unique capability can be run for HANE model scenarios and estimate potential radiation effects as needed.

Publications

Journal Articles

Engel, M. A., M. Cowee, V. K. Jordanova, G. S. Cunningham, Y. Chen and D. Larson. Simulation of the Formation and Evolution of an Artificial Belt of Ionized Fission Fragments. Submitted to *Journal of Radiation Effects Research and Engineering*. (LA-UR-20-23666)

Books/Chapters

Jordanova, V. K. CHAPTER 6: Ring Current Decay. (LA-UR-19-32034)

Reports

Chen, Y., M. A. Engel, V. K. Jordanova, M. Cowee, G. S. Cunningham and D. J. Larson. On the Radiation Effects of Strontium Ions on Satellite Solar Cells in Low Earth Orbits. Unpublished report. (LA-UR-21-20757)

Presentation Slides

Cowee, M. Artificial Radiation Belt Phenomenology Modeling. . (LA-CP-20-20502)

Cowee, M. Artificial Radiation Belts: Phenomenology and Modeling. . (LA-UR-20-27458)

Cowee, M. Artificial Radiation Belt Modeling at LANL. . (LA-UR-20-27529)

Cowee, M., V. K. Jordanova, M. A. Engel, Y. Chen and G. S. Cunningham. LANL LDRD Mission Foundations Project Update: Modeling an Artificial Radiation Belt of Ionized Fission Fragments After a HANE. . (LA-UR-20-30064)

Engel, M. A., M. Cowee, V. K. Jordanova, Y. Chen and G. S. Cunningham. Simulation of the Formation and Evolution of an Artificial Belt of Ionized Fission Fragments. Presented at *HEART*, Liousiville, Kentucky, United States, 2020-03-23 - 2020-03-27. (LA-UR-20-22361)

Posters

Engel, M. A., M. Cowee, V. K. Jordanova, S. K. Morley and M. G. Henderson. Impact of Loss Processes on Modeling the Ring Current. Presented at *American Geophysical Union*

How Can the Granular Defects of Additive Manufacturing be Evaluated?

Carly Donahue
20200495MFR

Project Description
Additive Manufacturing (AM) is currently revolutionizing fabrication of metal parts and is of growing importance in global security and weapons applications. This project will use novel techniques to analyze additively manufactured parts for defects. Department of Defense (DOD) and Department of Energy (DOE) weapons programs benefit from this work by allowing the parts to be non-destructively tested and verified to be of the required integrity before entering service. There are currently programs within the DOE weapons complex to do analysis of parts and determine what defects are problematic to material and part properties. Since inspection is an important part of technology and part qualification National Institute of Standards and Technology (NIST) is also working closely in these areas. National Aeronautics Space Administration (NASA) and the Federal Aviation Administration (FAA) are currently working on projects to accelerate adoption of AM-produced parts for aerospace applications. This research will have a significant impact on the ability to qualify a part for service in all industries. These defects are difficult if not impossible to detect through conventional non-destructive techniques making the proposed method very valuable.

Technical Outcomes
Additively Manufactured (AM) materials have complex microstructure that can affect the performance of a part if not well understood. This work has revealed with ultrasonic measurements that there is also signifcant anisotropy parallel to the build plate in AM materials. Additionally, resonant ultrasonic techniques, which are low-cost, nondestructive, and easy to implement, were shown to have measurables, including Poission ratio and hysteric nonlinearity, that correlated well with defect density, particularly undermelting defects.

Publications

Other

Donahue, C. M. and A. A. Bellotti. Dataset of nonlinear acoustics in granular material. Dataset. (LA-UR-21-26499)

Donahue, C. M. and C. J. Montgomery. Acoustic Data of Additively Manufactured Parts as part of LDRD MFR. Dataset. (LA-UR-20-23833)

Exploring Safeguard Signatures with Energy Resolved Neutron Imaging for Future Molten Salt Reactor Designs

Alexander Long
20210552MFR

Project Description

This project aims to address potential nuclear material accountancy and process monitoring issues in future domestic and international molten salt reactor designs. This project will explore energy-resolved neutron imaging (ERNI) capabilities as a potential material accountancy technique when applied to molten salts by performing several measurements at the Los Alamos Neutron Science Center (LANSCE) on various salt-actinide mixtures. The results will act at a small scale feasibility test and inform future efforts of possible technology gaps that need to be addressed in order to advance ERNI technology for safeguard proposes. If successful, further efforts and collaborations with industry partners and other Department of Energy (DOE) labs can advance and implement potential ERNI safeguard techniques in future designs, thus contributing to the overall success of fielding molten salt reactors (MSRs) both domestically and internationally.

Technical Outcomes

This project successfully achieved the main goal for providing capabilities to explore the energy-resolved neutron imaging (ERNI) applications as a material accountancy technique for future molten salt reactor (MSR) designs. New capabilities for ERNI measurements on Flight Path 5 (FP5) have been successfully deployed to allow for small scale feasibility testing on actinide-based salt mixtures. Additionally, a simulation framework has been developed to allow for the exploration and optimization of on-site ERNI measurements with initial results reported on high-assay low-enriched uranium (HALEU) based salts.

Publications

Presentation Slides

Horan, C. J. Novel Molten Salt Neutron Imaging Furnace Design. . (LA-UR-21-27092)

Horan, C. J. Generation IV Molten Salt Nuclear Reactors of the Future. . (LA-UR-21-27053)

Learning Fault Physics and Failure in Hydraulic Injection

Paul Johnson
20210561MFR

Project Description

Hydraulic injection is responsible for induced earthquakes, some of them damaging. For instance, in 2009 the Swiss Geothermal Program was terminated after an induced earthquake struck the project site beneath Basel, Switzerland. Indeed, large (>Magnitude 5.0) induced earthquakes from wastewater disposal related to hydraulic fracturing are common, often causing damage and regulatory changes. To date, a relatively crude approaches based on a 'stop light' has been the standard to address earthquake hazard. Our team has developed a data-driven, machine learning (ML) based approach to earthquake prediction. We have successfully developed ML models that can forecast earthquake failure time. The problem is that we cannot currently locate the signal, so in a region where multiple faults exist, it is challenging to know which fault may be slipping. That is the goal of our work. There is a strong benefit to missions in that we will markedly advance earthquake hazard in anthropogenic environments for application to energy reservoirs.

Technical Outcomes

This work advances earthquake hazards, by creating a deep learning tool that can be used for earthquake hazard assessment in both fluid-induced and tectonic earthquakes via a deep learning model that (1) automatically, rapidly identifies P and S-wave phases, (2) associates them with an earthquake, and then (3) locates the source. Such an approach could be used to assess materials of interest in an engineering or laboratory setting as well.

Publications

Presentation Slides

Johnson, P. A. and C. W. Johnson. Learning Fault Physics and Failure in Hydraulic Injection. . (LA-UR-21-25662)

Intelligent Coupling of X-ray Radiography and Acoustics for Accurate Rapid Assessments for Emergency Response

John Greenhall
20210563MFR

Project Description

Determining the geometry and materials of a sealed device is critical to determining what threat level that device poses and how to go about disablement. This determination is of great concern to National Nuclear Security Administration (NNSA) emergency response programs, and is currently an active field of research. Our proposed work integrates x-ray radiography and acoustic resonance spectroscopy to quickly measure the geometry and material configuration of a sealed system without disturbing the device. Alone, x-ray radiography is unable to distinguish between materials with similar densities, and acoustic resonance spectroscopy requires prior knowledge of the geometry to determine material properties. Thus, combining these techniques provides information that cannot be achieved by either method alone. In addition to emergency response, this technique would be beneficial in a range of different noninvasive measurement applications, including industrial process control, chemical reaction monitoring, and biomedical sensing.

Technical Outcomes

The project team acoustically and radiographically measured cubes of various materials and concentric shells with copper (Cu) outer and either tungsten (W) or tantalum (Ta) inner shells. The radiography showed little difference between the W and Ta cubes/shells, whereas the materials were easily differentiated based on acoustics. Additionally, the team compared the acoustic experimental measurements and numerical simulations with potential materials to identify specifically which material was present. This demonstrated how acoustic measurements enable material identification, where radiography alone does not.

Flight Software Framework for Agile Response to Global Security Threats

Markus Hehlen
20210701DI

Project Description

There is a need to deploy new space-based sensors on short timescales, for relatively low cost, and with high reliability. This level of mission agility is needed to (1) deliver actionable information on threat-relevant timescales, (2) significantly increase the cadence of developing and demonstrating new and resilient technologies in a relevant space environment, and (3) provide a framework for rapidly replenishing space assets in case of natural or manmade changes in the space environment. The two key enabling elements to create this capability are (1) leveraging commercial microsatellite technology for commodity components and services and (2) establishing a mission-agnostic technical and logistical framework that standardizes hardware, software, and workflows. The work proposed here focuses on the software component of this framework. We will develop a lean, mission-agnostic, and easy-to-maintain flight software framework that is architected and implemented specifically for microsatellite platforms. The results of this project will increase the mission agility of future microsatellite missions by streamlining the integration, testing, and operation of remote-sensing payloads. For Department of Energy/National Nuclear Security Administration, this work could enable more frequent on orbit tests and demonstrations of new sensor technology that will directly benefit the Space Nuclear Detonation Detection (SNDD) program.

Advanced Signatures, Processing, and Exploitation for Counter-proliferation (ASPEC)

Kevin Mitchell
20190651DI

Project Description

Remote sensing provides great operational value to the nonproliferation mission. Sensors must be regularly calibrated to ensure that their sensitivity is understood as they age. Existing calibration targets have limitations in their ability to support sensitivity calibration because of environmental uncertainties in the calibration scene. This project implements a new methodology for calibration target fabrication that removes the environmental uncertainties to create a new paradigm for sensor calibration. Additionally, existing analysis tools require significant subject matter expertise to use, and still do not effectively exploit all the information that is available. This project will explore the limits of the possible in remote sensing data analysis, and will develop analysis tools that can be used by non-specialists.

Technical Outcomes

This project was focused on developing new capabilities in the field of spectral remote sensing. Four tasks were supported: 1) next-generation spectral processing making use of recent advancements in machine learning, 2) new remote sensing calibration targets that eliminate environmental uncertainties, 3) tradecraft tools for non-specialists improving on state-of-the-art spectral information processing, and 4) detection of biological materials with spectral systems.

Publications

Reports

Duque, J. G., N. G. Parra-Vasquez, G. L. Wagner, L. R. Stromberg, H. Mukundan, J. J. Crochet and K. L. Mitchell. BETELGEUSE:Spectral Exploration of Biological Signatures for Remote Sensing Applications An LDRD-Director's Initiative. Unpublished report. (LA-CP-20-20299)

Presentation Slides

Duque, J. G., N. G. Parra-Vasquez, G. L. Wagner, J. J. Crochet and K. L. Mitchell. Detection and Identification of Biological Materials with Remote Sensing Techniques. . (LA-CP-20-20796)

Artificial Intelligence (AI)-Driven Collection and Models for Trust/Reliability of Integrated Space Surveillance Data

W Vestrand
20210702DI

Project Description

Once a high ground sanctuary for United States (US) national security assets, Space is now a war fighting domain that requires persistent, real-time, situational awareness. Starting with the Space Situational Awareness concept of full-sky persistent monitoring, anomaly detection, and autonomous real-time follow-up that was pioneered by our Thinking Telescopes project, we will build the foundations of a software testbed that will allow Los Alamos National Laboratory (LANL) to explore an extension of the concept to meet the emerging National Security issues associated with Space Surveillance. The central focus of our effort will be the construction of a virtual environment that will enable evaluation of a realistic, global scale, collection ecosystem. A key innovation of the global system concept is a new architecture, called a Dynamic Coalition Architecture, that employs Artificial Intelligence techniques to address the challenges associated with the collection of Space Surveillance measurements by a coalition of semi-autonomous government/commercial organizations. Altogether, this virtual testbed will enable the development of Artificial Intelligence controlled autonomous coordination, machine to machine sensor negotiation protocols, and exploration of trust/reliability modeling for data collected by realistic global Space Surveillance ecosystems.

Technical Outcomes

The team successfully developed a new concept for collaborative Space Traffic Management called a Dynamic Coalition Architecture that enables coordinated space surveillance by independent organizations. The architecture employs Artificial Intelligence techniques to organize sensors with different owner priorities into an efficient autonomous ecosystem that provides reliable real-time measurements. To quantify architecture effectiveness, the team created a virtual environment that simulates ecosystem management issues such as the real-time negotiation, sensor reliability and placement for optimal surveillance.

Publications

Conference Papers

Vestrand, W. T., P. R. Wozniak, S. M. Brennan, T. A. McVay, L. P. Parker, R. H. Sandoval and Y. H. Sechrest. Artificial Intelligence enabled Dynamic Coalition Architecture for Space Traffic Management. Presented at *AMOS 2021 Conference*. (Wailea, Hawaii, United States, 2021-09-14 - 2021-09-17). (LA-UR-21-28695)

Posters

Vestrand, W. T., P. R. Wozniak, S. M. Brennan, T. A. McVay, L. P. Parker, R. H. Sandoval and Y. H. Sechrest. Artificial Intelligence enabled Dynamic Coalition Architecture for Space Traffic Management. Presented at *AMOS 2021 Conference*, Wailea, Maui, Hawaii, United States, 2021-09-15 - 2021-09-17. (LA-UR-21-28822)

Scalable digital biosurveillance to advance pandemic science and preparedness

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20210767DI

Project Description

Infectious disease outbreaks, such as the coronavirus (COVID-19) pandemic this past year, have demonstrated the power of emerging infectious diseases to cause catastrophic harm to human health, overwhelm response capacities, and induce social, economic, and political upheaval. The COVID-19 pandemic has laid bare the extent to which the nation needs to improve their biosurveillance systems to detect and respond to the next pandemic or health crisis. This work will begin to address this National Security challenge by building a robust and standardized system that will track the State of New Mexico (as a regional example for the United States), for generating and collating genomic and epidemiologic data, and for performing the necessary analyses to identify new mutations and pandemic lineages of concern.

Technical Outcomes

Practical considerations for a scalable digital biosurveillance capability were successfully outlined with regional hospitals, diagnostic labs, universities and National Labs. Targeting SARS-CoV-2 detection, proof-of-concept studies to enhance throughput and reduce costs were performed on clinical and wastewater samples. These experimental methods detect other pathogens' signatures in multiple sample types, demonstrating preparedness for future pandemics/ outbreaks. Optimized SARS-CoV-2 genomic analyses include detection of variants of concern/interest and rapid incorporation of local data into a current global phylogeny.

Publications

Journal Articles

Hu, B., P. S. G. Chain, Y. Lin, P. Li and M. Babinski. SARS-CoV-2 variant phenotype prediction using genotype information. Submitted to *Molecular Systems Biology*. (LA-UR-22-20803)

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

Reports

Hu, B., J. D. Gans, Y. Lin, P. Li and P. S. G. Chain. Using Deep Mutational Data and Machine Learning to Guide Outbreak and Pandemic Response. Unpublished report. (LA-UR-22-21008)

Presentation Slides

Shakya, M. EDGE COVID-19: A web platform to generate submission-ready genomes from SARS-CoV-2 sequencing efforts. Presented at *International Conference on Infectious Diseases and Nanomedicine*, Kathmandu, Nepa, 2021-12-15 - 2021-12-15. (LA-UR-21-32266)

Posters

Kelliher, J. M., A. J. Hatch, A. J. Robinson, P. Li, K. W. Davenport, E. Hong-Geller and P. S. G. Chain. High-throughput pathogen detection and characterization in wastewater for SARS-CoV-2 and beyond. Presented at *SFAF*, Santa Fe, New Mexico, United States, 2021-09-28 - 2021-09-28. (LA-UR-21-29398)

Lo, C., M. Shakya, K. W. Davenport, M. C. Flynn, A. L. Myers y Gutierrez, P. Li, E. K. Player Jackson, B. Hu, Y. Xu and P. S. G. Chain. EDGE COVID-19: A Web Platform to generate submission-ready genomes from SARS-CoV-2 sequencing efforts.. Presented at *Sequencing to Function: Analysis and Application for the Futur*, Santa Fe, New Mexico, United States, 2021-09-28 - 2021-09-30. (LA-UR-21-28220)

Center for Space and Earth Science (CSES): Foundational Research in Space and Earth Science

Lisa Danielson
20210528CR-CSE

Project Description

This project provides national science research in the form of small, innovative, Research & Development (R&D) tasks in multidisciplinary physical sciences, along with pipelining and education opportunities that lead to filling critical roles within a wide range of national security programs within the Laboratory. The project is particularly responsive to the Department of Energy's Strategy to Advance American Space Leadership (FY 2021–FY 2031), "Energy for Space." Over half the project tasks support the three strategic goals, "Solve the Mysteries of Space," "Support the Secure and Peaceful Use of Space," and "Enable the Development of Space." This project supports space exploration via technology development and fundamental research that supports our understanding of the evolution of our universe, and also addresses our ability to model, analyze, and predict outcomes of potentially hazardous natural events on the Earth's surface or within the biome, enabling our ability to enhance our national climate and biosecurity.

Publications

Journal Articles

Fernando, B., N. W\xc3\xb3jcicka, M. Froment, R. Maguire, S. St\xc3\xa4hler, L. Rolland, G. S. Collins, O. Karatekin, C. Larmat, E. K. Sansom, N. A. Teanby, A. Spiga, F. Karakostas, K. Leng, T. Nissen-Meyer, T. Kawamura, D. Giardini, P. Lognonn\xc3\xa9, B. Banerdt and I. J. Daubar. Listening for the landing: Detecting Perseverance's landing with InSight.. Submitted to *Journal of Geophysical Research: Planets*. (LA-UR-20-29568)

Fernando, B., N. W\xc3\xb3jcicka, Z. Han, A. Stott, S. Ceylan, C. Charalambous, G. Collins, D. Est\xc3\xa9vez, M. Froment, M. Golombek, P. G\xc3\xbclzow, A. Horleston, O. Karatekin, T. Kawamura, C. Larmat, R. Maguire, T. Nissen-Meyer, M. Plasman, Y. Qia, L. Rolland, A. Spiga, N. A. Teanby, Y. S. Zhao, D. Giardini, P. Lognonn\xc3\xa9 and I. J. Daubar. Questions to Heaven. 2021. *Astronomy & Geophysics*. **62** (6): 6.22-6.25. (LA-UR-21-31668 DOI: 10.1093/astrogeo/atab103)

Goldberg, E. E., J. Hicks, D. Dinwiddie, D. Domman, C. McMullen, M. Sievers, D. Selvage and E. Romero-Severson. Case investigations and phylogenetics together reveal varied local transmission patterns of SARS-CoV-2. Submitted to *Epidemiology and Infection*. (LA-UR-21-23738)

Greess, S., J. Egedal, A. J. Stanier, W. S. Daughton, J. Olson, A. Y. Le, R. Myers, A. Millet-Ayala, M. Clark, J. Wallace, D. Endrizzi and C. Forest. Laboratory verification of electron-scale reconnection regions modulated by a three-dimensional instability. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-21-21878)

Guo, F., J. Giacalone and L. Zhao. Shock Propagation and Associated ParticleAcceleration in the Presence of AmbientSolar-Wind Turbulence. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-20-30411)

Harry, A., J. Drake, M. Swisdak, F. Guo, J. Dahlin, B. Chen, G. Fleishman, L. Glesener, K. Eduard, T. Phan and C. Shen. Electron Acceleration during Macroscale Non-Relativistic Magnetic Reconnection. Submitted to *Physical Review Letters*. (LA-UR-20-30073)

Karpov, P., I. Sitdikov, C. Huang and C. L. Fryer. Sapsan: Framework for Supernovae Turbulence Modeling with Machine Learning. Submitted to *Journal of Open Source Software*. (LA-UR-20-24238)

Karra, S., B. Ahmmed and M. Mudunuru. AdjointNet: Constraining machine learning models with physics-based codes. Submitted to *Journal of Computational Physics*. (LA-UR-21-28763)

Li, J., D. Lai and L. Rodet. Long-term evolution of Tightly-Packed Stellar Black Holes in AGN Disks: Formation of Merging Black-Hole Binaries via Close Encounters. Submitted to *Astrophysical Journal*. (LA-UR-22-22461)

Li, X., F. Guo and Y. Liu. The Acceleration of Charged Particles and Formation of Power-law Energy Spectra in Nonrelativistic Magnetic Reconnection. Submitted to *Physics of Plasmas*. (LA-UR-21-21365)

Lin, Y. and X. Zhang. Spatio-Temporal Graph Convolutional Networks for Earthquake Source Characterization.

Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-21-20806)

S. Mehana, M. Z., Q. Kang, H. S. Viswanathan and H. Nasrabadi. Molecular modeling of subsurface phenomena related to petroleum engineering. Submitted to *Earth Science Reviews*. (LA-UR-20-20902)

Ortiz, J. P., H. Rajaram, P. H. Stauffer, D. R. Harp, R. C. Wiens and K. W. Lewis. Venting deep subsurface methane via barometric pressure pumping: implications for life on Mars. Submitted to *Nature Geoscience*. (LA-UR-21-31710)

Ortiz, J. P., H. Rajaram, P. H. Stauffer, D. R. Harp, R. C. Wiens and K. W. Lewis. Supporting Information for "Venting deep subsurface methane via barometric pressure pumping: implications for life on Mars". Submitted to *Nature Geoscience*. (LA-UR-21-31944)

Ortiz, J. P., H. Rajaram, P. H. Stauffer, D. R. Harp, R. C. Wiens and K. W. Lewis. Barometric pumping through a fractured lithosphere: a mechanism for venting deep methane to Mars' atmosphere. Submitted to *Geophysical Research Letters*. (LA-UR-22-20869)

Ortiz, J. P., H. Rajaram, P. H. Stauffer, D. R. Harp, R. C. Wiens and K. W. Lewis. Supporting Information for "Barometric pumping through a fractured lithosphere: a mechanism for venting deep methane to Mars' atmosphere". Submitted to *Geophysical Research Letters*. (LA-UR-22-20882)

*. L. H. *. F. K. A. Sadler, J. D., J. D. Sadler, H. Li and K. A. Flippo. Parameter space for magnetization effects in high-energy-density plasmas. 2021. *Matter and Radiation at Extremes*. **6** (6): 65902. (LA-UR-21-23302 DOI: 10.1063/5.0057087)

Sadler, J. D., S. J. Green, S. Li, K. A. Flippo and H. Li. Faster ablative Kelvin-Helmholtz growth in a magnetic field. Submitted to *Physics of Plasmas*. (LA-UR-21-31295)

Sadler, J. D. and H. Li. Role of self-generated magnetic fields in the inertial fusion ignition threshold. Submitted to *Physical Review Letters*. (LA-UR-21-30942)

Walsh, C. A., J. D. Sadler and J. R. Davies. Impact of Updated Extended-MHD Transport Coefficients on Laboratory Plasmas. Submitted to *High Energy Density Physics*. (LA-UR-21-24909)

Zhang, H., X. Li, D. Giannios, F. Guo, Y. H. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–I. A. Submitted to *Astrophysical Journal*. (LA-UR-20-27998)

Zhang, Q., F. Guo, W. S. Daughton, X. Li and H. Li. Efficient Nonthermal Ion and Electron Acceleration Enabled by the Flux-Rope KinkInstability in 3D Nonrelativistic Magnetic Reconnection. Submitted to *Physical Review Letters*. (LA-UR-21-24459)

Zhang, Y., K. He, W. Li, G. Sun and S. McNulty. Detecting coastal wetland degradation by combining remote sensing and hydrologic modeling. Submitted to *Forest*. (LA-UR-22-21989)

zhang, h., X. Li, F. Guo and D. Giannios. First-Principle Prediction of X-ray Polarization from Magnetic Reconnection in High-Frequency BL Lacs. Submitted to *Astrophysical Journal Letters*. (LA-UR-20-30074)

Conference Papers

Froment, M., P. Lognonn\xc3\xa9, C. Larmat, E. Rougier, Z. Lei, T. Kawamura and F. Karakostas. Numerical Simulation of an Impact-Generated Stress-Glut Field and Corresponding Seismic Source. Presented at *52nd Lunar and Planetary Science Conference (LPSC 2021)*. (online, Texas, United States, 2021-03-15 - 2021-03-19). (LA-UR-21-21950)

Poulson, D. C., P. F. Bloser, K. Ogasawara, J. Trevino, J. S. Legere, J. M. Ryan and M. L. McConnell. Developing a Compton Telescope Prototype using Single-Crystal Diamond Detectors. Presented at *SPIE: Optics and Photonics*. (San Diego, California, United States, 2021-08-01 - 2021-08-05). (LA-UR-21-26844)

Ren, C. X., A. Ziemann, J. P. Theiler and J. S. Moore. Deepfaking-it: experiments in generative, adversarial multispectral remote sensing. Presented at *SPIE*. (Orlando, Florida, United States, 2021-04-12 - 2021-04-16). (LA-UR-21-23903)

Reports

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

McDanold, J. S. CSES_Chaos_FINALProposal. Unpublished report. (LA-UR-21-30490)

Ren, C. X., A. Ziemann, B. P. G. Rouet-Leduc, E. C. Reinisch and A. F. Roberts. Deep Learning for Sea Ice Characterization. Unpublished report. (LA-UR-21-21286)

Presentation Slides

Berner, A. M., P. J. Gasda, K. E. Mesick and C. Hardgrove. Exploring Gamma-Ray and Neutron Spectroscopy Missions to Mars Caves. . (LA-UR-21-27522)

Caldwell, W. K., A. Hunter and C. S. Plesko. Modeling Impacts on Rocky Asteroids for Potentially Hazardous Object Mitigation. Presented at *Center for Space and Earth Science Planetary Science Symposium*, Los Alamos, New Mexico, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-28046)

Caldwell, W. K., A. Hunter and C. S. Plesko. Benchmarking the FLAG Hydrocode for Kinetic Impactor Deflection Simulations. Presented at *Planetary Defense Conference*, Online, New Mexico, United States, 2021-04-26 - 2021-04-30. (LA-UR-21-23634)

Dolgopolova, E. and J. A. Hollingsworth. Controlled growth of metal-organic frameworks in gels. Presented at *ACS Spring Meeting 2021*, Online, New Mexico, United States, 2021-04-04 - 2021-04-30. (LA-UR-21-23396)

Engel, M. A. Development of Next-Generation Cross-Scale Equations for Magnetosphere Models. . (LA-UR-21-29914)

Evans, A. C. and M. B. Spano. Continuous Flow ISRU Biocatalytic Generation of Green Propellants for Space Travel. Presented at *CSES Biological Systems Symposium*, Los Alamos, New Mexico, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-29846)

Goldberg, E. E., E. Romero-Severson, D. Domman, D. Dinwiddie and J. Hicks. Transmission patterns of SARS-CoV-2 inferred from statistical phylogenetics and case investigations. Presented at *Quantitative Biology Colloquium, Univ Arizona*, Tucson (videocon), Arizona, United States, 2021-04-09 - 2021-04-09. (LA-UR-21-23235)

Guzik, J. A. A Tour of the Center of the Hertzsprung-Russell Diagram. . (LA-UR-21-30720)

Guzik, J. A., A. Baran, S. Sanjayan and P. Nemeth. Characterizing delta Scuti and gamma Doradus Variable Stars in the Kepler 'Superstamp' Field of Open Cluster NGC 6819. Presented at *110th Meeting of the American Association of Variable Star Observers*, Somerville, Massachusetts, United States, 2021-11-05 - 2021-11-07. (LA-UR-21-30702)

Karpov, P., C. Huang, C. L. Fryer and S. Iskandar. Sapsan: Framework for Supernovae Turbulence Modeling with Machine Learning. Presented at *SIAM CSE 21*, Online, Texas, United States, 2021-03-01 - 2021-03-05. (LA-UR-21-22091)

Koshkarov, O., G. L. Delzanno, V. Roytershteyn and C. Pagliantini. Reduced kinetic models for space physicsapplications. Presented at *Solar wind–Magnetosphere Interaction Workshop*, Online, New Mexico, United States, 2021-08-30 - 2021-08-30. (LA-UR-21-28668)

Larmat, C., L. Rolland and O. Karatekin. Modeling of the entry of Mars2020. Presented at *2021 CSES Planetary Symposia*, Online, New Mexico, United States, 2021-10-06 - 2021-10-06. (LA-UR-21-29901)

Li, H. A New Mechanism for the Ring and Spiral Formation in Protoplanetary Disks and Implications for Observations. Presented at *From cores to codes: planning for the next steps in planet formation*, Taipei, Taiwan, 2021-03-09 - 2021-03-09. (LA-UR-21-22171)

Li, H. A New Mechanism for the Ring and Spiral Formation in Protoplanetary Disks and Implications for Observations. . (LA-UR-21-23330)

Li, H. An AGN disk channel for binary black hole mergers. . (LA-UR-21-24829)

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

Neil, C. W., R. P. J. Hjelm, H. Xu, Y. Mao and J. Leao. Enhanced Oil Recovery from Tight Shale Probed by Small-angle Neutron Scattering Techniques Emulating Field Conditions. Presented at *2021 SSRL/LCLS Users Meeting*, Virtual Conference, New Mexico, United States, 2021-09-20 - 2021-09-24. (LA-UR-21-29316)

Nisbet, H. D. and A. Migdissov. REE in Hydrothermal Systems: From Ore Formation to Industrial Extraction. Presented at *CSES Geophysics Symposium*, Los Alamos, New Mexico, United States, 2021-10-04 - 2021-10-04. (LA-UR-21-29664)

Ortiz, J. P., P. H. Stauffer, R. C. Wiens, H. Rajaram and K. W. Lewis. Leveraging martian subsurface methane release data to inform models of gas release from clandestine nuclear testing. Presented at *Center for Space and Earth Science - Planetary Focus Area Symposium*, Webex, New Mexico, United States, 2021-10-06 - 2021-10-06. (LA-UR-21-29532)

Ortiz, J. P. and H. Rajaram. From Manhattan to Mars – Generating novel insights into methane fluctuations on the Red Planet. . (LA-UR-21-21723)

Pinilla-Orjuela, M. I. Autonomous Optimization for Pulsed Neutron Generators (PNGs). . (LA-UR-21-21736)

Pinilla-Orjuela, M. I. PiNG: The Interplanetary PNG Solution. Presented at *DisrupTECH 2021*, Los Alamos, New Mexico, United States, 2021-08-18 - 2021-08-18. (LA-UR-21-28165)

Rolland, L., E. Munaibari, F. Zedek, P. Sakic, A. Sladen, C. Larmat, D. T. Mikesell and B. Delouis. Worldwide GNSS ionospheric response analysis of the magnitude 8.8 2010 Chilean earthquake and tsunami: a revisit.. Presented at *EGU General Assembly 2021*, online, New Mexico, United States, 2021-04-19 - 2021-04-30. (LA-UR-21-23977)

Sadler, J. D., S. Li, S. Green, Y. Lu, K. A. Flippo, H. Li and C. A. Walsh. Symmetric theory of heat and magnetic transport in a collisional magnetized plasma. Presented at *American physical society division of plasma physics conference*, Pittsburgh, Pennsylvania, United States, 2021-11-08 - 2021-11-12. (LA-UR-21-30147)

S. Shin, T. H. The Search for Water on Planetary Bodies using Neutron Science. . (LA-UR-22-21910)

Simon, J. Modeling Gamma-ray and Neutron Spectroscopic Signatures in the Martian Subsurface. . (LA-UR-21-29604)

Solander, K. C. Other agency initiatives: remote sensing of Arctic sea ice and permafrost melt. . (LA-UR-22-22213)

Spano, M. B. and A. C. Evans. From Astronaut Urine to Rocket Fuel. Presented at *UCI Group Meeting - Greg Weiss Group*, Irvine, California, United States, 2021-08-16 - 2021-08-16. (LA-UR-21-28151)

Konakondula Vydula, A., D. D. S. Coupland, K. E. Mesick, B. P. Weaver and C. Hardgrove. Measurement of Neutron Lifetime Using a Space-based Neutron Spectrometer. Presented at *LANL Student Symposium*, Online, New Mexico, United States, 2021-08-03 - 2021-08-04. (LA-UR-21-27570)

Posters

Berner, A. M., S. Czarnecki, C. Hardgrove, P. J. Gasda and K. E. Mesick. Measuring Hydration of Nearby Cliffs in Gale Crater Using Neutron Observations. Presented at *Lunar*

and Planetary Science Conference, The Woodlands, Texas, United States, 2022-03-07 - 2022-03-11. (LA-UR-22-21845)

Li, J., A. M. Dempsey, H. Li and S. Li. Ring Formation in Protoplanetary Discs Driven by an Eccentric Instability. Presented at *Distorted Astrophysical Discs: New Insights and Future Directions*, Online, New Mexico, United States, 2021-05-17 - 2021-05-20. (LA-UR-21-24581)

Poulson, D. C., P. F. Bloser, D. Kim, K. Ogasawara, J. Trevino, J. S. Legere, J. M. Ryan and M. L. McConnell. A Prototype Compton Telescope using Singe-Crystal Diamond Detectors. Presented at *IEEE NSS/MIC*, Online, New Mexico, United States, 2021-10-16 - 2021-10-23. (LA-UR-21-30192)

Poulson, D. C., P. F. Bloser, K. Ogasawara, J. Trevino, J. S. Legere, J. M. Ryan and M. L. McConnell. Developing a Compton Telescope Prototype using Single-Crystal Diamond Detectors. Presented at *SPIE: Optics and Photonics*, San Diego, California, United States, 2021-08-01 - 2021-08-05. (LA-UR-21-26843)

Rolland, L., E. Munaibari, C. Larmat, T. D. Mikesell, A. Sladen, B. Delouis and P. Lognonn\xc3\xa9. The Resonant Ionospheric Response of the Magnitude 8.8 2010 Chilean Earthquake. Presented at *2021 AGU Fall meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31937)

Other

Daughton, W. S. Challenges and Opportunities for Understanding Magnetic Reconnection in Large Systems. Audio/Visual. (LA-UR-21-26838)

Larmat, C. MarsIntaSeis Notebook. Dataset. (LA-UR-20-29840)

Emerging Challenges in Space and Earth Science

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20180475CR-CSE

Project Description

This project provides national science research & education services that benefit a wide range of Los Alamos National Laboratory's national security programs in global security, energy and climate security and space situational awareness, and the modeling capability in the stockpile stewardship program. This includes university research outreach and student / postdoc research programs, which are the technical heart of this project. This project further provides funding for new ideas and programs that may play a large part in the future DOE/NNSA mission. Support for innovative small work also plays a large role in the Lab's retention of technical talent.

Technical Outcomes

The project consisted of many smaller tasks in Astrophysics, Space Science, Planetary Science, Earth Systems, and Geophysics, all peer reviewed and aligned with Laboratory strategy. The project focused heavily on Workforce Development via student/postdoc involvement, now at the Laboratory (no longer online). Around 50% of the funded postdocs, Chick Keller Fellows, will transition to staff. The project supported 78 tasks, which delivered results at a remarkable rate, including 84 publications and 129 conference presentations.

Publications

Journal Articles

*Abeysekara, A. U., A. Albert, R. Alfaro, C. Alvarez, R. Arceo, J. C. Arteaga-Velazquez, D. A. Rojas, H. A. A. Solares, E. Belmont-Moreno, S. Y. BenZvi, C. Brisbois, K. S. Caballero-Mora, A. Carraminana, S. Casanova, J. Cotzomi, S. C. de Leon, C. De Leon, E. De la Fuente, S. Dichiara, B. L. Dingus, M. A. DuVernois, J. C. Diaz-Velez, K. Engel, C. Espinoza, H. Fleischhack, N. Fraija, A. Galvan-Gamez, J. A. Garcia-Gonzalez, M. M. Gonzalez, J. A. Goodman, J. P. Harding, B. Hona, F. Hueyotl-Zahuantitla, P. Huntemeyer, A. Iriarte, A. Lara, W. H. Lee, H. L. Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, J. Lundeen, K. Malone, S. S. Marinelli, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, J. A. Matthews, P. Miranda-Romagnoli, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, M. U. Nisa, R. Noriega-Papaqui, E. G. Perez-Perez, Z. Ren, C. D. Rho, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, H. Salazar, F. S. Greus, A. Sandoval, M. Schneider, G. Sinnis, A. J. Smith, R. W. Springer, K. Tollefson, I. Torres, G. Vianello, T. Weisgarber, J. Wood, T. Yapici, A. Zepeda, H. Zhou and J. D. Alvarez. Searching for dark matter sub-structure with HAWC. 2019. *Journal of Cosmology and Astroparticle Physics*. **2019** (07): 022. (LA-UR-18-31168 DOI: 10.1088/1475-7516/2019/07/022)

*Albert, A., R. Alfaro, C. Alvarez, J. R. Angeles Camacho, J. C. Arteaga-Velazquez, K. P. Arunbabu, D. Avila Rojas, H. A. A. Solares, V. Baghmanyan, E. Belmont-Moreno, S. Y. BenZvi, C. Brisbois, K. S. Caballero-Mora, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. Coutino de Leon, E. De la Fuente, C. de Leon, B. L. Dingus, M. A. DuVernois, J. C. Diaz-Velez, R. W. Ellsworth, K. Engel, C. Espinoza, H. Fleischhack, N. Fraija, A. Galvan-Gamez, D. Garcia, J. A. Garcia-Gonzalez, F. Garfias, M. M. Gonzalez, J. A. Goodman, J. P. Harding, S. Hernandez, B. Hona, D. Huang, F. Hueyotl-Zahuantitla, P. Huntemeyer, A. Iriarte, V. Joshi, A. Lara, W. H. Lee, H. Leon Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, J. Lundeen, R. Lopez-Coto, K. Malone, S. S. Marinelli, I. Martinez-Castellanos, J. Martinez-Castro, H. Martinez-Huerta, J. A. Matthews, P. Miranda-Romagnoli, J. A. Morales-Soto, E. Moreno, A. Nayerhoda, L. Nellen, M. Newbold, M. U. Nisa, R. Noriega-Papaqui, N. Omodei, A. Peisker, E. G. Perez-Perez, C. D. Rho, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, E. Ruiz-Velasco, H. Salazar, F. S. Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, G. Sinnis, A. J. Smith, R. W. Springer, P. Surajbali, E. Tabachnick, M. Tanner, O. Tibolla, K. Tollefson, I. Torres, R. Torres-Escobedo, T. Weisgarber, G. Yodh, A. Zepeda and H. Zhou. Constraints on Lorentz Invariance Violation from HAWC Observations of Gamma Rays above 100\xc2\xa0TeV. 2020. *Physical Review Letters*. **124** (13): 131101. (LA-UR-21-22669 DOI: 10.1103/PhysRevLett.124.131101)

*Banerjee, T., T. Holland, K. Solander, M. Holmes and R. Linn. Identifying Characteristics of Wildfire Towers and Troughs. 2020. *Atmosphere*. **11** (8): 796. (LA-UR-19-30049 DOI: 10.3390/atmos11080796)

Begeman, C. B., X. S. Asay-Davis and L. Van Roekel. Ice-shelf ocean boundary layer dynamics from large-

eddy simulations. Submitted to *The Cryosphere*. (LA-UR-21-27878)

*Bonneville, A., R. Kouzes, J. Yamaoka, A. Lintereur, J. Flygare, G. S. Varner, I. Mostafanezhad, E. Guardincerri, C. Rowe and R. Mellors. Borehole muography of subsurface reservoirs. 2018. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*. **377** (2137): 20180060. (LA-UR-18-26169 DOI: 10.1098/rsta.2018.0060)

*Bonneville, A., R. T. Kouzes, J. Yamaoka, C. Rowe, E. Guardincerri, J. M. Durham, C. L. Morris, D. C. Poulson, K. Plaud-Ramos, D. J. Morley, J. D. Bacon, J. Bynes, J. Cercillieux, C. Ketter, K. Le, I. Mostafanezhad, G. Varner, J. Flygare and A. T. Lintereur. A novel muon detector for borehole density tomography. 2017. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **851**: 108-117. (LA-UR-16-27062 DOI: 10.1016/j.nima.2017.01.023)

S. Boyce, S. H., Z. Lei, B. J. Euser, E. E. Knight, E. Rougier, J. Stormont and M. Reda-Taha. Simulation of mixed-mode fracture using the combined finite–discrete element method. 2020. *Computational Particle Mechanics*. **7** (5): 1047-1055. (LA-UR-19-32443 DOI: 10.1007/s40571-020-00341-6)

*Caldwell, W. K., A. Hunter, C. S. Plesko and S. Wirkus. Understanding Asteroid 16 Psyche's composition through 3D impact crater modeling. 2020. *Icarus*. **351**: 113962. (LA-UR-19-32428 DOI: 10.1016/j.icarus.2020.113962)

Caldwell, W. K., A. Hunter and C. S. Plesko. Exploring Porosity in Asteroid 16 Psyche with 3D Hydrocode Modeling of Its Deepest Impact Structure. Submitted to *Icarus*. (LA-UR-21-30361)

Chen, G., H. Fu, Y. Zhang, X. Li, Y. Ge, A. Du, C. Liu and Y. Xu. Energetic Electron Acceleration in Unconfined Reconnection Jets. Submitted to *Astrophysical Journal Letters*. (LA-UR-19-28967)

*Chen, Y., G. D. Reeves, G. S. Cunningham, R. J. Redmon and M. G. Henderson. Forecasting and remote sensing outer belt relativistic electrons from low Earth orbit. 2016. *Geophysical Research Letters*. **43** (3): 1031-1038. (LA-UR-15-27476 DOI: 10.1002/2015GL067481)

*Chen, Y., G. D. Reeves, X. Fu and M. Henderson. PreMevE: New Predictive Model for Megaelectron-Volt Electrons Inside Earth's Outer Radiation Belt. 2019. *Space Weather*. **17** (3): 438-454. (LA-UR-18-29269 DOI: 10.1029/2018SW002095)

*Cosburn, K., M. Roy, E. Guardincerri and C. Rowe. Joint inversion of gravity with cosmic ray muon data at a well-characterized site for shallow subsurface density prediction. 2019. *Geophysical Journal International*. **217** (3): 1988-2002. (LA-UR-18-23891 DOI: 10.1093/gji/ggz127)

Cote, B., M. Eichler, A. Yague, N. Vassh, M. R. Mumpower, B. Vilagos, B. Soos, A. Arcones, T. M. Sprouse, R. Surman,

M. Pignatari, B. Wehmeyer, T. Rauscher and M. Lugaro. Constraining the rapid neutron-capture process with meteoritic 129-I and 247-Cm. Submitted to *Science*. (LA-UR-19-30942)

Curtis, S., N. M. Lloyd Ronning, J. M. Miller and C. Frohlich. Full Transport GRRMHD for Kilonovae from Black Hole—Neutron Star Merger Disks. Submitted to *Astrophysical Journal*. (LA-UR-20-27560)

Curtis, S., N. Wolfe, C. Frohlich, J. M. Miller, R. T. Wollaeger, K. Ebinger and A. Perego. Supernova Lightcurves and Spectra. Submitted to *Astrophysical Journal*. (LA-UR-20-26099)

*Czarnecki, S., C. Hardgrove, P. J. Gasda, T. S. Gabriel, M. Starr, M. Rice, J. Frydenvang, R. C. Wiens, W. Rapin, S. Nikiforov, D. Lisov, M. Litvak, F. Calef, H. Gengl, H. Newsom, L. Thompson and S. F. Nowicki. Identification and Description of a Silicic Volcaniclastic Layer in Gale Crater, Mars, Using Active Neutron Interrogation. 2020. *Journal of Geophysical Research: Planets*. **125** (3): e2019JE006180. (LA-UR-19-26619 DOI: 10.1029/2019JE006180)

*Dra\xc5\xbckowska, J., S. Li, T. Birnstiel, S. M. Stammler and H. Li. Including Dust Coagulation in Hydrodynamic Models of Protoplanetary Disks: Dust Evolution in the Vicinity of a Jupiter-mass Planet. 2019. *The Astrophysical Journal*. **885** (1): 91. (LA-UR-20-28594 DOI: 10.3847/1538-4357/ab46b7)

Dra\xcc\xa7\xc5\xbckowska, J., S. Li, T. Birnstiel, S. M. Stammler and H. Li. Including Dust Coagulation in Hydrodynamic Models of Protoplanetary Disks: Dust Evolution in the Vicinity of a Jupiter-mass Planet. Submitted to *Astrophysical Journal*. (LA-UR-19-30949)

*Froment, M., E. Rougier, C. Larmat, Z. Lei, B. Euser, S. Kedar, J. E. Richardson, T. Kawamura and P. Lognonne. Lagrangian-based Simulations of Hypervelocity Impact Experiments on Mars Regolith Proxy. 2020. *Geophysical Research Letters*. **47** (13): e2020GL087393. (LA-UR-19-32642 DOI: 10.1029/2020GL087393)

Froment, M., E. Rougier, C. Larmat, Z. Lei, B. J. Euser, S. Kedar, J. E. Richardson, T. Kawamura and P. Lognonne. Supporting Information for "Lagrangian-based simulations of hypervelocity impact experiments on Mars regolith proxy". Submitted to *Geophysical Research Letters*. (LA-UR-20-22081)

*Gehring, C., S. A. Sevanto, A. Patterson, D. Ulrich and C. R. Kuske. Ectomycorrhizal and Dark Septate Fungal Associations of Pinyon Pine Are Differentially Affected by Experimental Drought and Warming. 2020. *Frontiers in Plant Science*. **11**: 582574. (LA-UR-20-25014 DOI: 10.3389/fpls.2020.582574)

*Goodsman, D. W., G. J. Grosklos, B. H. Aukema, C. Whitehouse, K. Bleiker, N. G. McDowell, R. S. Middleton and C. Xu. The effect of warmer winters on the demography of an outbreak insect is hidden by intraspecific competition. 2018. *Global Change Biology*. (LA-UR-17-30013 DOI: 10.1111/gcb.14284)

*Greess, S., J. Egedal, A. Stanier, W. Daughton, J. Olson, A. Le, R. Myers, A. Millet-Ayala, M. Clark, J. Wallace, D. Endrizzi and C. Forest. Laboratory Verification of Electron-Scale Reconnection Regions Modulated by a Three-Dimensional Instability. 2021. *Journal of Geophysical Research: Space Physics*. **126** (7). (LA-UR-20-24836 DOI: 10.1029/2021JA029316)

*Guo, F., X. Li, W. Daughton, P. Kilian, H. Li, Y. Liu, W. Yan and D. Ma. Determining the Dominant Acceleration Mechanism during Relativistic Magnetic Reconnection in Large-scale Systems. 2019. *Physical Review Letters*. **879** (2). (LA-UR-18-31752 DOI: 10.3847/2041-8213/ab2a15)

Guo, F., X. Li, W. S. Daughton, H. Li, P. F. H. Kilian, Y. H. Liu, Q. Zhang and H. Zhang. Magnetic Energy Release, Plasma Dynamics and Particle Acceleration during Relativistic Turbulent Magnetic Reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-26005)

*Guo, F., Y. Liu, X. Li, H. Li, W. Daughton and P. Kilian. Recent progress on particle acceleration and reconnection physics during magnetic reconnection in the magnetically-dominated relativistic regime. 2020. *Physics of Plasmas*. **27** (8): 080501. (LA-UR-20-26135 DOI: 10.1063/5.0012094)

Guzik, J. A. Highlights of Discoveries for \xe1\xba\x9f Scuti Variable Stars from the Kepler Era. Submitted to *Frontiers in Astronomy and Space Sciences*. (LA-UR-21-20345)

Hagengruber, T. L., M. M. Reda Taha, E. Rougier, E. E. Knight and J. C. Stormont. Failure in confined Brazilian tests on sandstone. Submitted to *Applied Sciences*. (LA-UR-21-21150)

Hagengruber, T. L., M. Reda Taha, E. Rougier, E. E. Knight and J. C. Stormont. Evolution of permeability in sandstone during confined Brazilian testing. Submitted to *Rock Mechanics and Rock Engineering*. (LA-UR-20-30383)

Harding, J. P. and J. A. Lundeen. A Search For Dark Matter Signals in the GalacticHalo with HAWC. Submitted to *PoS - Proceedings of Science*. (LA-UR-21-22676 DOI: 10.22323/1.358.0528)

Holmbeck, E., A. Frebel, G. C. McLaughlin, R. Surman, R. Fernandez, B. D. Metzger, M. R. Mumpower and T. M. Sprouse. Reconstructing masses of merging neutron stars from stellar r-process abundance signatures. Submitted to *Astrophysical Journal*. (LA-UR-20-27862)

*Holmes, R. M. and D. M. Palmer. Extreme background-rejection techniques for the ELROI optical satellite license plate. 2019. *Applied Optics*. **58** (4): 814. (LA-UR-18-28957 DOI: 10.1364/AO.58.000814)

*Hunter, A., B. A. Moore, M. Mudunuru, V. Chau, R. Tchoua, C. Nyshadham, S. Karra, D. O'Malley, E. Rougier, H. Viswanathan and G. Srinivasan. Reduced-order modeling through machine learning and graph-theoretic approaches for brittle fracture applications. 2019. *Computational Materials Science*. **157**: 87-98. (LA-UR-18-29900 DOI: 10.1016/j.commatsci.2018.10.036)

*Johnson, P. A., J. Carmeliet, H. M. Savage, M. Scuderi, B. M. Carpenter, R. A. Guyer, E. G. Daub and C. Marone. Dynamically triggered slip leading to sustained fault gouge weakening under laboratory shear conditions. 2016. *Geophysical Research Letters*. **43** (4): 1559-1565. (LA-UR-15-29118 DOI: 10.1002/2015GL067056)

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

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

*Kilian, P., X. Li, F. Guo and H. Li. Exploring the Acceleration Mechanisms for Particle Injection and Power-law Formation during Transrelativistic Magnetic Reconnection. 2020. *The Astrophysical Journal*. **899** (2): 151. (LA-UR-20-20135 DOI: 10.3847/1538-4357/aba1e9)

Kroeniger, K., F. De Roo, P. Brugger, S. Huq, T. Banerjee and M. Mauder. Effect of Secondary Circulations on the Surface–Atmosphere Exchange of Energy at an Isolated Semi-arid Forest. 2018. *Boundary-Layer Meteorology*. (LA-UR-17-30829 DOI: 10.1007/s10546-018-0370-6)

*Kunegel-Lion, M., D. W. Goodsman and M. A. Lewis. When managers forage for pests: Implementing the functional response in pest management. 2019. *Ecological Modelling*. **396**: 59-73. (LA-UR-17-30015 DOI: 10.1016/j.ecolmodel.2018.10.013)

*Li, H. Meso-scale Instability Triggered by Dust Feedback in Dusty Rings: Origin and Observational Implications. 2020. *Astrophysical Journal*. **893** (2): 89. (LA-UR-20-20221 DOI: 10.3847/1538-4357/ab8199)

*Li, J., A. M. Dempsey, H. Li and S. Li. Ring Formation in Protoplanetary Disks Driven by an Eccentric Instability. 2021. *The Astrophysical Journal*. **910** (1): 79. (LA-UR-20-27570 DOI: 10.3847/1538-4357/abe1b6)

*Li, J., D. Lai, K. R. Anderson and B. Pu. Giant planet scatterings and collisions: hydrodynamics, merger-ejection branching ratio, and properties of the remnants. 2021. *Monthly Notices of the Royal Astronomical Society*. **501** (2): 1621-1632. (LA-UR-20-24165 DOI: 10.1093/mnras/staa3779)

*Li, J. and D. Lai. Planetary Spin and Obliquity from Mergers. 2020. *The Astrophysical Journal*. **898** (1): L20. (LA-UR-20-23627 DOI: 10.3847/2041-8213/aba2c4)

*Li, Y., H. Li, S. Li and D. N. C. Lin. On the Dust Signatures Induced by Eccentric Super-Earths in Protoplanetary Disks. 2019. *The Astrophysical Journal*. **886** (1): 62. (LA-UR-19-27695 DOI: 10.3847/1538-4357/ab4bc8)

*Lin, Y. Data-Driven Seismic Waveform Inversion: A Study on the Robustness and Generalization. 2020. *IEEE Transactions on Geoscience and Remote Sensing*. **58** (10): 6900-6913. (LA-UR-19-24398 DOI: 10.1109/TGRS.2020.2977635)

Lin, Y. Earthquake Detection in 1-D Time Series Data with Feature Selection and Dictionary Learning. Submitted to *Seismological Research Letters*. (LA-UR-19-31060)

Lin, Y., J. P. Theiler and B. E. Wohlberg. Physics-Consistent Data-driven Waveform Inversion with Adaptive Data Augmentation. Submitted to *IEEE Geoscience and Remote Sensing Letters*. (LA-UR-20-22488)

Lin, Y., Z. Zhang, T. Chen, Y. Wu and A. A. Delorey. Earthquake Detection Using Convolutional Neural Networks: Deep VS Shallow Nets?. Submitted to *Seismological Research Letters*. (LA-UR-18-29645)

Lin, Y. and Y. Wu. InversionNet: A Real-Time and Accurate Full Waveform Inversion with CNNs and continuous CRFs. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-18-30679)

Lu, Y., C. Huang, P. F. H. Kilian, F. Guo, H. Li and E. P. Liang. An O(N) and semi-implicit Maxwell solver with improved numerical dispersion properties. Submitted to *Computer Physics Communications*. (LA-UR-19-27359)

Lu, Y., C. Huang, P. F. H. Kilian, F. Guo, H. Li and E. P. Liang. Time step dependent force interpolation scheme for relativistic particle-in-cell simulations. Submitted to *Journal of Computational Physics*. (LA-UR-19-29419)

Lu, Y., F. Guo, P. F. H. Kilian, H. Li, C. Huang and E. P. Liang. Fermi-type particle acceleration from magnetic reconnection at the termination shock of a relativistic striped wind. Submitted to *Astrophysical Journal*. (LA-UR-20-27625)

Lundeen, J. A. "Dark Matter in the Galactic Halo with HAWC". Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30003)

Lundeen, J. A. "Dark Matter Searches with HAWC". Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30002)

Mellors, R., C. A. Rowe, G. Chapline, A. Bonneville, R. Kouzes, E. Guardincerri and N. Bonal. Muons and seismic: a dynamic duo for the shallow subsurface?. 2016. *FastTIMES*. **21** (4): 24-28. (LA-UR-16-28664)

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

Mottola, E. and A. Sadofyev. Chiral Waves on the Fermi-Dirac Sea. Submitted to *Physical Review Letters*. (LA-UR-18-29339)

*Mudunuru, M. K., N. Panda, S. Karra, G. Srinivasan, V. T. Chau, E. Rougier, A. Hunter and H. S. Viswanathan. Surrogate Models for Estimating Failure in Brittle and Quasi-Brittle Materials. 2019. *Applied Sciences*. **9** (13): 2706. (LA-UR-18-25370 DOI: 10.3390/app9132706)

Mudunuru, M. K., V. Chillara, S. Karra and D. N. Sinha. Scalable Time Series Feature Engineering Framework to Understand Multiphase Flow using Acoustic Signals. Submitted to *Proceedings of Meetings of Acoustics, 172nd ASA Meeting - Honolulu*. (LA-UR-18-20456)

Nisbet, H. D., A. Migdissov, A. E. Williams-Jones, V. van Hinsberg, H. Xu and R. C. Roback. The solubility of thorium in carbonate-bearing solutions at hydrothermal conditions. 2021. *Geochimica et Cosmochimica Acta*. (LA-UR-20-30269 DOI: 10.1016/j.gca.2021.04.035)

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

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

Padilla, A. M., M. A. Najvani, E. E. Knight, E. Rougier, J. Stormont and M. M. Reda Taha. Correlating Damage and Cracking with Air Permeability in Concrete Using the Brazilian Tension Test. Submitted to *Construction and Building Materials*. (LA-UR-21-31931)

Padilla, A., M. Genedy, E. E. Knight, E. Rougier, J. Stormont and M. Reda Taha. A New Stiff Brazilian Tension Test for Monitoring Post-Peak Crack Propagation in Concrete and Brittle Rock Materials. Submitted to *Cement and Concrete Research*. (LA-UR-20-21120)

Paris, M. W., V. Cirigliano and S. M. Shalgar. Collective neutrino oscillations with the halo effect in single-angle approximation. Submitted to *Journal of Cosmology and Astroparticle Physics*. (LA-UR-19-20928)

*Ren, C. X., O. Dorostkar, B. Rouet-Leduc, C. Hulbert, D. Strebel, R. A. Guyer, P. A. Johnson and J. Carmeliet. Machine Learning Reveals the State of Intermittent Frictional Dynamics in a Sheared Granular Fault. 2019. *Geophysical Research Letters*. **46** (13): 7395-7403. (LA-UR-19-22300 DOI: 10.1029/2019GL082706)

Rougier, E., A. Munjiza and J. Munjiza. Distributed intelligence and the equivalence of matter and information. 2020. *Computational Particle Mechanics*. **7** (5): 1073-1080. (LA-UR-20-20345 DOI: 10.1007/s40571-020-00340-7)

*Roy, M., M. Lewis, A. Johnson, N. George, C. Rowe and E. Guardincerri. Inferring Shallow Subsurface Density Structure from Surface and Underground Gravity Measurements: Calibrating Models for Relatively Undeformed Volcanic Strata at the Jemez Volcanic Field,

New Mexico, USA. 2018. *Pure and Applied Geophysics*. **175** (3): 1003-1018. (LA-UR-17-26322 DOI: 10.1007/s00024-017-1742-4)

Salvesen, G. M. and J. M. Miller. Black Hole Spin in X-ray Binaries: Giving Uncertainties an f. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-20-28487)

Sevanto, S. A., C. Still, A. M. Sibley, G. Page and F. Meinzer. Temperature biases from instrument designs: a caution about inferring leaf thermoregulation from gas exchange measurements. Submitted to *Agricultural and Forest Meteorology*. (LA-UR-18-30732)

*M. M. *. S. R. Sprouse, T. *., T. M. Sprouse and M. R. Mumpower. Following Fission Products in Explosive Astrophysical Environments. *EPJ Web of Conferences*. **242**: 4001. (LA-UR-20-21940 DOI: 10.1051/epjconf/202024204001)

. M. M. R. *. S. R. Sprouse, T. M., T. M. Sprouse and M. R. Mumpower. Following nuclei through nucleosynthesis: A novel tracing technique. 2021. *Physical Review C*. **104 (1): 015803. (LA-UR-20-24018 DOI: 10.1103/PhysRevC.104.015803)

*Still, C. J., A. Sibley, G. Page, F. C. Meinzer and S. Sevanto. When a cuvette is not a canopy: A caution about measuring leaf temperature during gas exchange measurements. 2019. *Agricultural and Forest Meteorology*. **279**: 107737. (LA-UR-19-30645 DOI: 10.1016/j.agrformet.2019.107737)

Still, C., G. Page, D. M. Griffith, B. Rastogi, D. M. Aubrecht, Y. Kim, S. Burns, C. V. Hanson, H. Kwon, F. C. Meinzer, S. A. Sevanto, D. Roberts, M. Goulden, S. Pau, M. Detto, B. R. Helliker and A. D. Richardson. Continuous, long-term leaf temperature data from diverse forest types do not support the leaf homeothermy hypothesis. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-24466)

*M. Ulrich, D. E., S. Sevanto, S. Peterson, M. Ryan and J. Dunbar. Effects of Soil Microbes on Functional Traits of Loblolly Pine (Pinus taeda) Seedling Families From Contrasting Climates. 2020. *Frontiers in Plant Science*. **10**. (LA-UR-19-31097 DOI: 10.3389/fpls.2019.01643)

Ulrich, D., S. A. Sevanto, M. G. Ryan, M. B. N. Albright, R. Johansen and J. M. Dunbar. Plant-microbe interactions before drought influence plant physiological responses to subsequent severe drought. Submitted to *Nature Scientific Reports*. (LA-UR-19-30513)

*Vesselinov, V. V., M. K. Mudunuru, S. Karra, D. O'Malley and B. S. Alexandrov. Unsupervised machine learning based on non-negative tensor factorization for analyzing reactive-mixing. 2019. *Journal of Computational Physics*. **395**: 85-104. (LA-UR-18-20868 DOI: 10.1016/j.jcp.2019.05.039)

*Vira, A. D., P. A. Fernandes, H. O. I. Funsten, S. K. Morley, H. Yamaguchi, F. Liu and N. A. Moody. Angular scattering of protons through ultrathin graphene foils: Application for time-of-flight instrumentation. 2020. *Journal of Geophysical Research: Space Physics*. **91** (3): 033302. (LA-UR-19-24967 DOI: 10.1063/1.5134768)

*Vira, A. D., P. A. Fernandes, R. M. Skoug, H. O. Funsten and D. B. Reisenfeld. Understanding Mass Resolution of Foil-Based Time-of-Flight Mass Spectrometry. 2020. *Journal of Geophysical Research: Space Physics*. **125** (8): e2020JA027971. (LA-UR-20-20898 DOI: 10.1029/2020JA027971)

Wang, X., B. D. Fields, M. R. Mumpower, T. M. Sprouse, R. Surman and N. Vassh. Sandblasting the r-process: spallation of ejecta from neutron star mergers. Submitted to *Astrophysical Journal*. (LA-UR-19-29391)

. L. J. J. *. R. E. J. *. O. D. M. *. K. C. M. *. M. S. K. Welling, D. T. and S. K. Morley. Numerical Simulations of the Geospace Response to the Arrival of an Idealized Perfect Interplanetary Coronal Mass Ejection. 2020. *Space Weather*. **19 (2): e2020SW002489. (LA-UR-20-27454 DOI: 10.1029/2020SW002489)

*Yuan, B., Y. J. Tan, M. K. Mudunuru, O. E. Marcillo, A. A. Delorey, P. M. Roberts, J. D. Webster, C. N. L. Gammans, S. Karra, G. D. Guthrie and P. A. Johnson. Using Machine Learning to Discern Eruption in Noisy Environments: A Case Study Using CO2-Driven Cold-Water Geyser in Chimay\xc3\xb3, New Mexico. 2019. *Seismological Research Letters*. **90** (2A): 591-603. (LA-UR-18-29261 DOI: 10.1785/0220180306)

*Zhou, Z., Y. Lin, Z. Zhang, Y. Wu, Z. Wang, R. Dilmore and G. Guthrie. A data-driven CO2 leakage detection using seismic data and spatial–temporal densely connected convolutional neural networks. 2019. *International Journal of Greenhouse Gas Control*. **90**: 102790. (LA-UR-18-29329 DOI: 10.1016/j.ijggc.2019.102790)

Conference Papers

Boyce, S., J. Stormont, M. Reda-Taha, Z. Lei, B. J. Euser, E. E. Knight and E. Rougier. Simulation of Mixed-mode Failure in Carrara Marble using the Combined Finite-Discrete Element Method. Presented at *ARMA 2019*. (New York City, New York, United States, 2019-06-23 - 2019-06-26). (LA-UR-19-21765)

Dong, B., P. F. H. Kilian, X. Li, F. Guo, S. Byna and K. Wu. Terabyte-scale Particle Data Analysis: An ArrayUDF Case Study. Presented at *SSDBM 2019 : 31st International Conference on Scientific & Statistical Database Management*. (Santa Cruz, California, United States, 2019-07-23 - 2019-07-25). (LA-UR-19-24098)

Guzik, J. A., J. Jackiewicz, A. Pigulski, G. Catanzaro, M. S. Soukup, P. Gaulme and G. Handler. Data Analysis of Bright Main-Sequence A- and B-type Stars Observed Using the TESS and BRITE Spacecraft. Presented at *Society of Astronomical Sciences Symposium (to be held on-line)*. (Ontario, California, United States, 2020-05-30 - 2020-06-21). (LA-UR-20-23732)

Guzik, J. A., J. Jackiewicz, G. Catanzaro and M. S. Soukup. Characterizing Variability in Bright Metallic-Line A (Am) Stars Using Data from the NASA TESS Spacecraft. Presented at *Society for Astronomical Sciences Annual Symposium*. (online conference, California, United States, 2021-06-15 - 2021-06-22). (LA-UR-21-25150)

Hagengruber, T., E. Rougier, E. E. Knight, B. J. Euser, M. M. Taha and J. C. Stormont. Gas permeability measurements during confined Brazilian testing. Presented at *54th US Rock Mechanics / Geomechanics Symposium*. (Golden, Colorado, United States, 2020-06-28 - 2020-06-28). (LA-UR-20-21973)

Holmbeck, E., R. Surman, A. Frebel, G. C. McLaughlin, M. R. Mumpower, T. M. Sprouse, T. Kawano, N. Vassh and T. C. Beers. Characterizing r-process sites through actinide production. Presented at *Nuclear Physics in Astrophysics IX*. (Frankfurt, Germany, 2019-09-15 - 2019-09-15). (LA-UR-20-22074)

Holmes, R. M., C. T. Weaver and D. Palmer. ELROI: A satellite license plate to simplify space object identification. Presented at *Advanced Maui Optical Surveillance (AMOS) conference 2018*. (Wailea, Hawaii, United States, 2018-09-10 - 2018-09-14). (LA-UR-18-28191)

Holmes, R. M., S. J. Gill, J. Z. Harris, J. S. Lansford, W. R. Myers, C. T. Weaver, A. Zucherman, A. Jorgensen and D. Palmer. Status of ELROI satellite license plate demonstration on the CubeSat NMTSat. Presented at *SPIE Defense + Commercial Sensing*. (Baltimore, Maryland, United States, 2019-04-15 - 2019-04-15). (LA-UR-19-22913)

Karpov, P., I. Sitdikov, C. Huang and C. L. Fryer. Sapsan: Framework for Supernovae Turbulence Modeling with Machine Learning. Presented at *Conference on Neural Information Processing Systems (NeurIPS 2020)*. (Vancouver, Canada, 2020-12-06 - 2020-12-12). (LA-UR-20-24238)

I. Lewellen, J. W., L. R. Danielson, A. Essunfeld, J. A. Hollingsworth, M. A. Holloway and E. K. Lewis. KARVE: A NANOPARTICLE ACCELERATOR FOR SPACE THRUSTER APPLICATIONS. Presented at *12th International Particle Accelerator Conference*. (Campinas, Brazil, 2021-05-24 - 2021-05-24). (LA-UR-21-24895)

Leyba, J., C. Rusch, E. Rougier, E. E. Knight, B. J. Euser, J. Stormont and M. Reda Taha. Modelling the significance of a rubber sleeve on the indirect tensile strength of concrete. Presented at *2nd International Discrete Fracture Network Engineering Conference*. (Seattle, Washington, United States, 2018-06-20 - 2018-06-20). (LA-UR-18-22740)

Lin, Y. VelocityGAN: Subsurface Velocity Image Estimation Using Conditional Adversarial Networks. Presented at *IEEE Winter Conf. on Applications of Computer Vision*. (Waikoloa Village, Hawaii, United States, 2019-01-08 - 2019-01-08). (LA-UR-18-29102)

Lin, Y. Full-waveform Inversion with Applications to Subsurface Characterization and Breast Cancer Detection. Presented at *Society of Exploration Geophysics Annual Meeting*.

(houston, Texas, United States, 2020-10-11 - 2020-10-11). (LA-UR-20-22876)

Lin, Y., P. Li and E. S. Schultz-Fellenz. ENCODED HOURGLASS NETWORK FOR SEMANTIC SEGMENTATION OF HIGH RESOLUTION AERIAL IMAGERY. Presented at *the International Conference on Acoustics, Speech, and Signal Processing*. (Brighton, United Kingdom, 2019-05-12 - 2019-05-12). (LA-UR-18-30682)

Lin, Y., Z. Zhang, Z. Zhou and T. Chen. ADAPTIVE FILTERING FOR EVENT RECOGNITION FROM NOISY SIGNAL: AN APPLICATION TO EARTHQUAKE DETECTION. Presented at *International Conference on Acoustics, Speech, and Signal Processing*. (Brighton, United Kingdom, 2019-05-12 - 2019-05-12). (LA-UR-18-30687)

Lin, Y. and N. Sha. Efficient seismic denoising techniques using robust principal component analysis. Presented at *seg*. (San Antonio, Texas, United States, 2019-09-16 - 2019-09-16). (LA-UR-19-22983)

Lin, Y. and R. A. Pires de Lima. Transforming seismic data into pseudo-RGB images to predict CO2 leakage using pre-learned convolutional neural networks weights. Presented at *SEG*. (San Antonio, Texas, United States, 2019-09-16 - 2019-09-16). (LA-UR-19-22979)

Lin, Y. and T. Wang. EarthquakeGen: Earthquake Generator Using Generative Adversarial Networks. Presented at *seg*. (San Antonio, Texas, United States, 2019-09-16 - 2019-09-16). (LA-UR-19-22982)

Lu, Y., F. Guo, P. F. H. Kilian, H. Li, C. Huang and E. P. Liang. Studying particle acceleration from driven magnetic reconnection at the termination shock of a relativistic striped wind using particle-in-cell simulations. Presented at *49th International Symposium on Multiparticle Dynamics*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-13). (LA-UR-20-22375)

Miars, G., B. E. Gilchrist, O. Leon and G. L. Delzanno. Parameters Impacting Ion Emission from a Contactor Plasma. Presented at *6th international conference on tethers in space*. (Madrid, Spain, 2019-06-12 - 2019-06-12). (LA-UR-19-30104)

Pinilla-Orjuela, M. I., P. F. Bloser, J. R. Tutt, K. E. Mesick, S. F. Nowicki, M. R. Mumpower and R. S. Miller. A Lunar CubeSat mission for high-sensitivity nuclear astrophysics. Presented at *SPIE Astronomical Telescopes and Instrumentation*. (Online, New Mexico, United States, 2020-12-14 - 2020-12-18). (LA-UR-20-29830)

Rusch, C., J. Leyba, E. E. Knight, E. Rougier, J. Stormont and M. Reda Taha. Measuring apparent air permeability of concrete during Brazilian tension test. Presented at *52nd US Rock Mechanics/Geomechanics Symposium*. (Seattle, Washington, United States, 2018-06-17 - 2018-06-17). (LA-UR-18-22481)

Vassh, N., M. R. Mumpower, T. M. Sprouse and R. Surman. Probing the properties of neutron-rich actinides with

the astrophysical r process. Presented at *International Workshop on Fission Product Yields*. (Santa Fe, New Mexico, United States, 2019-09-30 - 2019-09-30). (LA-UR-20-22730)

Reports

Barthel, A. M. Final report for IC project w20_soheat "High-resolution Southern Ocean heat transport modeling to better quantify uncertainties in future Antarctic melt". Unpublished report. (LA-UR-21-24333)

Carlsten, B. E. Final Report "1-MeV Accelerator-in-Space Design" Center for Space and Earth Science R&D Project. Unpublished report. (LA-UR-19-25097)

Connor, R., J. R. Brister, J. P. Buchmann, W. Deboutte, R. A. Edwards, J. Marti-Carreras, M. Tisza, V. Zalunin, J. S. Andrade-Martinez, V. A. Cantu, M. R. D'Amour, A. Efremov, L. Fleischmann, L. M. Forero-Junco, S. Garmaeva, M. Giluso, C. Glickman, M. Henderson, B. P. Kellman, D. M. Kristensen, C. Leubsdorf Jr., K. Levi, S. Levi, S. B. Pakala, V. Peddu, A. J. Ponsero, E. Ribeiro, F. M. Roy, L. Rutter, S. Saha, M. Shakya, R. Shean, M. A. Miller, B. J. Tully, C. J. R. Turkington, K. Youens-Clark, B. Vanmechelen and B. Busby. NCBI's Virus Discovery Hackathon: Engaging Research Communities to Identify Cloud Infrastructure Requirements. Unpublished report. (LA-UR-19-27395)

D'Angelo, G., E. C. Hunke, T. R. Pitts, S. F. D. Price and A. F. Roberts. Sea ice evolution along the Northern Sea Route and implications for trans-Arctic shipping from 2021 through 2060. Unpublished report. (LA-UR-21-31464)

Froment, M. Mid-Term report : Seismic Modeling of Meteorite Impacts on the Surface of Mars. Unpublished report. (LA-UR-20-21855)

Holmes, R. M. Aeon essay (untitled draft). Unpublished report. (LA-UR-19-23345)

H. Kilian, P. F. Consequences of Yee latice on diagnostics. Unpublished report. (LA-UR-19-24116)

Mumpower, M. R., O. Korobkin, J. M. Miller and T. M. Sprouse. Nuclear Data for Astrophysics on the Eve of FRIB. Unpublished report. (LA-UR-20-26586)

Rani, B., H. Zhang, S. Hunter, F. Kislat, M. Boettcher, J. E. McEnery, D. Giannios, F. Guo, H. Li, M. G. Baring, I. Agudo, S. Buson, M. Petropoulou, V. Pavlidou, E. Angelakis, I. Myserlis, Z. Wadiasingh, R. Curado da Silva, P. F. H. Kilian, S. Guiriec, V. Bozhilov, S. Anton, M. Kazana, P. Coppi, T. M. Venters, F. Longo and E. Bottacini. High-Energy Polarimetry - a new window to probe extreme physics in AGN jets. Unpublished report. (LA-UR-19-22708)

Rougier, E., E. E. Knight, J. C. Stormont and M. Reda Taha. The Large University Project 2017-2020 Sponsored by CSES and NMC Correlating Damage, Fracture and Permeability in Rocks subjected to High Strain Rate Loading. Unpublished report. (LA-UR-21-21974)

Schreiner, C., P. F. H. Kilian, F. Spanier, P. Mu\xc3\xb1oz and J. Buechner. Ion acceleration in non-relativistic quasi-parallel shocks using fully kinetic simulations. Unpublished report. (LA-UR-20-22389)

Woodroffe, J. R., V. E. Bernstein, A. C. Walker, L. M. Winter, S. Chakraborty, S. K. Morley, X. Liu, V. K. Jordanova, M. A. Engel, B. A. Larsen, P. A. Fernandes, M. Shumko, M. R. Carver, A. M. Wold, X. Fu, M. Cowee, L. Woodham, F. Guo and T. Singh. 2018 Los Alamos Space Weather Summer School Research Reports. Unpublished report. (LA-UR-18-31636)

Presentation Slides

Banerjee, T. and R. R. Linn. Effect of canopy architectural variation on transpiration and thermoregulation. Presented at *AGU 2017*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-30830)

Banerjee, T. and R. R. Linn. How trees uptake carbon, release water and cool themselves in air: a marriage between biophysics and turbulent fluid dynamics. Presented at *APS DFD*, Denver, Colorado, United States, 2017-11-19 - 2017-11-21. (LA-UR-17-30727)

Barthel, A. M. High-resolution Southern Ocean heat transport modeling to better quantify uncertainties in future Antarctic melt. . (LA-UR-21-24334)

Begeman, C. B. Changing climate\xc2\xa0and melting ice: perspectives from field work and climate modeling. . (LA-UR-21-25976)

Begeman, C. B., X. S. Asay-Davis and L. Van Roekel. Toward a new ice-shelf melt rate parameterization with large-eddy simulations. Presented at *EGU General Assembly 2020*, Online, New Mexico, United States, 2020-05-04 - 2020-05-08. (LA-UR-20-23270)

Begeman, C. B., X. S. Asay-Davis and L. Van Roekel. Turbulent controls on ice-shelf melting. . (LA-UR-20-27773)

Blaschke, D. Neutrino Quantum Kinetic Equations: The Collision Term. Presented at *NBIA-LANL Neutrino Quantum Kinetics in Dense Environments*, Copenhagen, Denmark, 2019-08-26 - 2019-08-26. (LA-UR-19-28605)

S. Boyce, S. H. An Experimental Study Correlating Damage and Permeability in Brittle Geo-Materials using Confined, Flattened Brazilian Disks.. Presented at *Coffee and Geophysics*, Los Alamos, New Mexico, United States, 2020-02-27 - 2020-02-27. (LA-UR-20-21882)

Caldwell, W. K. Impact Simulations. Presented at *Graduate Seminar*, Tempe, Arizona, United States, 2019-03-12 - 2019-03-12. (LA-UR-19-22010)

Caldwell, W. K. Differential Equation Models for Understanding Phenomena beyond Experimental Capabilities. Presented at *Graduate Seminar*, Tempe, Arizona, United States, 2019-03-12 - 2019-03-12. (LA-UR-19-22015)

Caldwell, W. K. Differential Equation Models for Understanding Phenomena beyond Experimental Capabilities. Presented at *Collaboration meeting*, Glendale, Arizona, United States, 2019-04-11 - 2019-04-11. (LA-UR-19-23204)

Caldwell, W. K. FLAG Hydrocode. . (LA-UR-19-23662)

Caldwell, W. K. Modeling Crater Formation. Presented at *2019 Summer Physics Camp for Young Women*, Pojaque, New Mexico, United States, 2019-06-13 - 2019-06-13. (LA-UR-19-25404)

Caldwell, W. K. Rubble Pile Modeling of Asteroid 16 Psyche. Presented at *DART IT Meeting (online, remote access)*, Mesa, Arizona, United States, 2020-05-12 - 2020-05-12. (LA-UR-20-23530)

Caldwell, W. K. Planetary Defense: Saving the World through Science (Eventually). Presented at *WESST Fest Virtual Powerwall Tour*, Los Alamos, New Mexico, United States, 2020-09-01 - 2020-09-01. (LA-UR-20-26574)

Caldwell, W. K. Simulating Asteroid Impacts for Forthcoming NASA Missions. Presented at *Math Will Save the World Seminar*, Tempe, Arizona, United States, 2020-09-02 - 2020-09-02. (LA-UR-20-26790)

Caldwell, W. K. Making an Impact: One Scientist's Unusual Career Path. Presented at *Capital High School (virtual STEM outreach)*, Virtual, New Mexico, United States, 2020-10-09 - 2020-10-09. (LA-UR-20-27990)

Caldwell, W. K. Space Rocks on Earth and Beyond. Presented at *Earth Week 2021*, Online, New Mexico, United States, 2021-04-19 - 2021-04-22. (LA-UR-21-23635)

Caldwell, W. K. DART Inverse 2 in FLAG: Challenges Presented and Lessons Learned. Presented at *DART Investigation Team Meeting*, Mesa, Arizona, United States, 2021-06-14 - 2021-06-17. (LA-UR-21-25527)

Caldwell, W. K., A. Hunter, C. S. Plesko and S. Wirkus. Understanding Asteroid 16 Psyche's Composition through 3D Hydrocode Impact Crater Models. Presented at *Joint Mathematics Meeting*, Denver, Colorado, United States, 2020-01-16 - 2020-01-16. (LA-UR-20-20398)

Caldwell, W. K., A. Hunter and C. S. Plesko. Modeling Impacts on Rocky Asteroids for Potentially Hazardous Object Mitigation. Presented at *Center for Space and Earth Science Planetary Science Symposium*, Los Alamos, New Mexico, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-28046)

Caldwell, W. K., A. Hunter and C. S. Plesko. Benchmarking the FLAG Hydrocode for Kinetic Impactor Deflection Simulations. Presented at *Planetary Defense Conference*, Online, New Mexico, United States, 2021-04-26 - 2021-04-30. (LA-UR-21-23634)

Caldwell, W. K., M. A. Buechler, A. Hunter and C. S. Plesko. (U) Code Implementation for Subterranean and Extraterrestrial Applications. Presented at *NECDC 2021*, Online, New Mexico, United States, 2021-05-10 - 2021-05-14. (LA-CP-21-20341)

Chen, Y. A New Predictive Model for Relativistic Electrons in Outer Radiation Belt. Presented at *AGU 2017 Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-30906)

Chen, Y. Listen to the Canary: Understanding and Utilizing a Storm Precursor in Low-Earth-Orbits for MeV Electrons in the Earth's Radiation Belt. . (LA-UR-18-29728)

Chen, Y. Insights into Dynamics of Earth's Electron Radiation Belts from Precipitation Observations. Presented at *Breckenridge Workshop 2017*, Breckenridge, Colorado, United States, 2017-05-22 - 2017-05-26. (LA-UR-17-24184)

Chen, Y. PreMevE: A Neural Network Based Predictive Model for MeV Electrons inside Earth's Outer Radiation Belt. Presented at *Space Weather Workshop 2019*, Boulder, Colorado, United States, 2019-04-02 - 2019-04-05. (LA-UR-19-23013)

Chen, Y., X. Fu, G. D. Reeves and M. G. Henderson. PreMevE: A New Predictive Model for Megaelectron-volt Electrons inside Earth's Outer Radiation Belt. Presented at *15th European Space Weather Week*, Leuven, Belgium, 2018-11-05 - 2018-11-09. (LA-UR-18-30426)

Collins, A. D. and A. M. Sibley. Adaptation of Juniper and Pi \xc3\xb1on Pine to high temperature in the Survival Mortality experiment (SUMO). Presented at *CSES (Earth Systems) Symposium*, Los Alamos, New Mexico, United States, 2019-08-21 - 2019-08-21. (LA-UR-19-28393)

S. Coupland, D. D., K. E. Mesick and C. D. Roecker. Analysis of Lunar Prospector Data to Constrain the Neutron Lifetime. . (LA-UR-18-29883)

Curtis, S., J. M. Miller, R. T. Wollaeger, C. Frohlich and N. Wolfe. Core-collapse Supernovae: From Neutrino-Driven 1D Explosions to Light Curves and Spectra. . (LA-UR-20-26964)

DeMets, S. A., K. C. Solander, C. A. Manore and S. Y. Del Valle. Mosquito tracking using data from the upcoming NASA SWOT Mission. Presented at *Center for Earth and Space Science, Earth Systems Symposium*, Los Alamos, New Mexico, United States, 2020-10-02 - 2020-10-02. (LA-UR-20-27716)

Dolgopolova, E. and J. A. Hollingsworth. Shooting for the Stars: Opening New Dimensions for Metal-Organic Frameworks. Presented at *Center for Space and Earth Science Symposium*, Los Alamos, New Mexico, United States, 2020-10-26 - 2020-10-26. (LA-UR-20-28567)

Dorfman, S., V. Roytershteyn, B. Van Compernolle, C. A. Cattell, G. L. Delzanno, B. E. Carlsten and K. Nichols. Experimental Investigation of Wave Generation by an Electron Beam in Magnetized Plasma. Presented at *APS DPP*, Portland, Oregon, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-31033)

Evans, A. C. Continuous Flow Biocatalytic Production of Green Propellant Fuel from Biowaste for Deep Space Travel. . (LA-UR-20-28188)

Froment, M. How hard should Mars be hit to unravel its hidden history?. . (LA-UR-20-21486)

Froment, M. Shock wave modeling for the Impact Working Group. . (LA-UR-20-21560)

Froment, M. How hard should Mars be hit to unravel its hidden history?. . (LA-UR-20-23649)

Froment, M. Simulation of CMBD impacts. . (LA-UR-20-24596)

Froment, M. Seismic Modeling of Meteorite Impacts on the Surface of Mars.. . (LA-UR-20-26615)

Froment, M. Simulation of the CMBD impacts. . (LA-UR-20-27069)

Froment, M. E\xcc\x81tude comparative de la source sismique des impacts de me\xcc\x81te\xcc\x81orites a\xcc\x80 la surface de diffe\xcc\x81rents corps.. . (LA-UR-21-24732)

Froment, M. Simulating Seismic Signals of Meteorite Impacts with the Finite-Discrete Element Method.. Presented at *Particles2021*, Hamburg, Germany, 2021-10-04 - 2021-10-06. (LA-UR-21-29676)

Froment, M. Numerical simulations of meteorite impacts, towards a new source model. Presented at *MAGIS ANR meeting*, Toulouse, France, 2021-11-22 - 2021-11-23. (LA-UR-21-31346)

Froment, M. The Seismic Source of a Meteorite Impact. . (LA-UR-22-20902)

Froment, M., E. Rougier, C. Larmat, Z. Lei, B. J. Euser, S. Kedar, J. Richardson, T. Kawamura and P. Lognonn\xc3\xa9. Lagrangian-based simulations of hypervelocity impact experiments on Mars regolith proxy. Presented at *18th Science Meeting Insight*, Pasadena, California, United States, 2020-07-20 - 2020-07-24. (LA-UR-20-25363)

Froment, M., P. Lognonn\xc3\xa9, C. Larmat, E. Rougier, Z. Lei, T. Kawamura and F. Karakostas. Numerical Simulation of an Impact-Generated Stress-Glut Field and Corresponding Seismic Source. Presented at *NASA / InSight Science Team Meeting 20*, Online, New Mexico, United States, 2021-03-08 - 2021-03-12. (LA-UR-21-22169)

Froment, M. and C. Larmat. How hard should Mars be hit to unravel its hidden history ?. . (LA-UR-21-29555)

Goodsman, D. W. Will a warmer climate impact how we monitor and manage mountain pine beetle populations?. . (LA-UR-18-23519)

Guzik, J. A., A. Pigulski, P. Gaulme and G. Handler. BRITE observations of four targets in the 38-Cyg-III-2018 field and comparison with Kepler and TESS data. Presented at *BRITE Meeting*, Online, Austria, 2021-07-12 - 2021-07-12. (LA-UR-21-26823)

Guzik, J. A., J. Jackiewicz, A. Pigulski, G. Catanzaro, M. S. Soukup, P. Gaulme and G. Handler. Analysis of Bright Star Data from the TESS and BRITE Spacecraft. Presented at *Society of Astronomical Sciences Symposium*, Online (Ontario), California, United States, 2020-05-30 - 2020-06-21. (LA-UR-20-24259)

Harding, J. P. HAWC Dark Matter Searches. Presented at *MAGIC Dark Matter workshop*, Barcelona, Spain, 2019-01-16 - 2019-01-17. (LA-UR-19-20300)

Hiraki, K. DREAM results with Arase, Himawari, and GPS. . (LA-UR-20-20423)

Holmes, R. M. ELROI: A license plate for satellites that anyone can read. Presented at *Small Satellite Conference*, Logan, Utah, United States, 2018-08-04 - 2018-08-09. (LA-UR-18-26945)

Holmes, R. M. Space traffic management & why satellites need license plates. . (LA-UR-18-31379)

Holmes, R. M. Status of ELROI satellite license plate demonstration on the CubeSat NMTSat. Presented at *SPIE Defense + Commercial Sensing*, Baltimore, Maryland, United States, 2019-04-14 - 2019-04-18. (LA-UR-19-23303)

Huang, C. and G. Pilania. Adaptive autonomic closure for the plasma transport problem. . (LA-UR-18-22548)

Hunke, E. C. The Arctic LDRD project: What happened?. . (LA-UR-20-29636)

Johnson, E., C. Hardgrove, K. E. Mesick, G. Stoddard, J. F. Christian, M. E. Kaffine, L. Heffern, J. Dubois, B. Roebuck, N. Struebel, I. Lazbin, P. Hailey, T. Prettyman and R. Starr. Characterization of the LunaH-Map Miniature Neutron Spectrometer. Presented at *IEEE Nuclear Science Symposium*, Virtual, New Mexico, United States, 2020-10-31 - 2020-10-31. (LA-UR-20-29223)

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

H. Kilian, P. F. Numerical Plasma Physics. . (LA-UR-20-23604)

H. Kilian, P. F., X. Li, F. Guo and H. Li. How magnetic reconnection injects particles and accelerates them to high energies. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-22043)

H. Kilian, P. F., X. Li, F. Guo and H. Li. Exploring the acceleration mechanisms for particle injection and power-law formation during trans-relativistic magnetic reconnection. Presented at *Understanding the Most Energetic Cosmic Accelerators: Advances in Theory and Simulation*, Online, New Mexico, United States, 2020-10-28 - 2020-10-30. (LA-UR-20-28623)

Kintner, J. A. Advancements in Local-Distance Relative Seismic Event Location, Magnitude Estimation, and the Association of Seismic Wave Arrivals - A Case Study of Industrial Blasting Practices in the Powder River Basin, Wyoming. Presented at *External Review, LANL GNDD Source Physics*, Los Alamos, New Mexico, United States, 2020-09-15 - 2020-09-15. (LA-UR-20-27032)

Kintner, J. A., N. P. Symons, J. K. MacCarthy and J. D. Carmichael. Formulating the Seismic Association Problem Using Graph Theory, Applications to Estimating an Efficient Solution with Quantum Computers. Presented at *AGU 2020*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29391)

Kintner, J. A., N. P. Symons, J. K. MacCarthy and J. D. Carmichael. Formulating the Seismic Association Problem Using Graph Theory, Applications to Estimating an Efficient Solution with Quantum Computers. Presented at *AGU Fall Meeting*, Virtual, New Mexico, United States, 2020-12-01 - 2020-12-17. (LA-UR-20-29680)

Knight, E. E., E. Rougier and S. H. S. Boyce. HOSS Selected Simulation Examples. . (LA-UR-20-26164)

Larmat, C., E. Rougier and M. Froment. How hard should Mars be hit to unravel its hidden history?. Presented at *2020 CSES Planetary Science Consortium*, Los ALamos, New Mexico, United States, 2020-10-13 - 2020-10-13. (LA-UR-20-28140)

I. Lewellen, J. W., L. R. Danielson, A. Essunfeld, J. A. Hollingsworth, M. A. Holloway and E. Lewis. KARVE: A Nanoparticle Accelerator for Space Thruster Applications. Presented at *12th International Particle Accelerator Conference – IPAC 2021*, Campinas, Brazil, 2021-05-24 - 2021-05-24. (LA-UR-21-24685)

Li, Y., H. Li, S. Li, L. Ricci, D. Lin, T. Birnstiel, A. Isella, M. Ansdell, F. Yuan, J. Drazkowska and S. Stammler. Ringed Structures and Dust Growth in Protoplanetary Disks. Presented at *XXXI IUPAP Conference on Computational Physics*, Hong Kong, China, 2019-07-28 - 2019-08-01. (LA-UR-19-23594)

Lin, Y., Y. Wu, Z. Zhou, A. A. Delorey and T. Chen. Geyser Detection with Deep Densely Connected Network. Presented at *SIAM Data Mining Meeting*, San Diego, California, United States, 2018-05-03 - 2018-05-05. (LA-UR-18-26578)

Lin, Y., Z. Zhongping, Y. Wu, P. A. Johnson and Z. Zhou. Earthquake Detection in 1-D Time Series Data with Feature Selection and Dictionary Learning. Presented at *SIAM Data Mining Meeting*, San Diego, California, United States, 2018-05-03 - 2018-05-05. (LA-UR-18-26576)

Lu, Y., C. Huang, P. F. H. Kilian, F. Guo, H. Li and E. P. Liang. Development of a O(N) Maxwell solver with improved numerical dispersion properties. Presented at *26th International Conference on Numerical Simulation of Plasma*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28794)

Lu, Y., C. Huang, P. F. H. Kilian, F. Guo, H. Li and E. P. Liang. New methods for suppressing numerical Cherenkov instability in relativistic particle-in-cell simulations. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30615)

Lu, Y., F. Guo, H. Li and E. P. Liang. Fermi-type particle acceleration from magnetic reconnection at the termination shock of relativistic striped wind. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30620)

Lundeen, J. A. Dark Matter in the Galactic Halo with HAWC. Presented at *APS April Meeting*, Denver, Colorado, United States, 2019-04-13 - 2019-04-13. (LA-UR-19-30006)

Lundeen, J. A. "Dark Matter in the Galactic Halo with HAWC". Presented at *International Cosmic Ray Conference*, Wisconsin, Wisconsin, United States, 2019-07-24 - 2019-07-24. (LA-UR-19-30004)

Lundeen, J. A. Dark Matter Searches with HAWC. Presented at *International Cosmic Ray Conference*, Madison, Wisconsin, United States, 2019-07-24 - 2019-07-24. (LA-UR-19-30005)

Marias, D. E. The carbon cost of plant-microbe interactions under climate change. Presented at *Science in "3"*, Los Alamos, New Mexico, United States, 2018-06-13 - 2018-06-13. (LA-UR-18-24320)

Mauney, C. M., I. Sagert and W. P. Even. Changes in Atmospheric Chemistry due to Asteroid Impacts on Earth. Presented at *CSES Earth Systems Symposium*, Los Alamos, New Mexico, United States, 2019-08-21 - 2019-08-21. (LA-UR-19-30393)

Mesick, K. E. Engagement in LunaH-Map Mini-NS Detector Calibration. . (LA-UR-18-30099)

Migdissov, A., X. Guo, H. D. Nisbet, N. F. van Hartesveldt, A. Kalintsev, H. Xu, H. Boukhalfa, R. C. Roback, V. van Hinsberg, A. E. Williams-Jones, R. I. Gabitov and J. Brugger. Geochemical controls of mobilisation, deposition, and fractionation of REE, U, and Th in ore forming hydrothermal systems. Presented at *Goldschmidt 2018*, Boston, Massachusetts, United States, 2018-08-12 - 2018-08-18. (LA-UR-18-27542)

Migdissov, A. and H. D. Nisbet. REE in Hydrothermal Systems: From Ore Formation to Industrial Extraction. Presented at *Center for Space and Earth Science Geophysics Symposium*, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-12. (LA-UR-20-28218)

Miller, J. M. Neutrinos: The Ghosts From Space. . (LA-UR-20-26425)

Miller, J. M., S. Curtis and N. M. Lloyd Ronning. Blue Kilonova From Black Hole-Neutron Star Disks. Presented at *CSES Astrophysics Symposium*, Los Alamos, New Mexico, United States, 2020-10-01 - 2020-10-01. (LA-UR-20-27535)

Morley, S. K. Physics-Based Modeling of Space Weather During Large and Extreme Geomagnetic Storms. . (LA-UR-21-21997)

Morley, S. K., S. M. Graf and D. T. Welling. Reconstructing and Modeling a Benchmark Space Weather Event. Presented at *Center for Space and Earth Science Space*

Symposium, Online, New Mexico, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-28013)

Mudunuru, M. K. EDGEip - Intelligent Processing at the Edge to Enhance Efficiency. . (LA-UR-18-22222)

Mudunuru, M. K. Forecasting CO2-driven cold-water geyser eruptions using machine learning. Presented at *CSES talk*, Los Alamos, New Mexico, United States, 2018-10-30 - 2018-10-30. (LA-UR-18-30348)

Mudunuru, M. K. EDGEip - Intelligent Processing at the Edge to Enhance Efficiency. . (LA-UR-19-29757)

Mudunuru, M. K. IoGES: Internet of Things for Geophysical and Environmental Sensing. . (LA-UR-19-30467)

Mudunuru, M. K., S. Karra, V. V. Vesselinov, J. Reddy and K. Naksahtrala. Machine learning and reduced-order models for complex systems. Presented at *WCCM XIII/PANACM II Minisymposium Session Proposal, 2018*, New York, New York, United States, 2018-07-22 - 2018-07-27. (LA-UR-18-21880)

Mudunuru, M. K., V. Chillara, S. Karra and D. N. Sinha. A machine learning framework to understand multiphase flow using acoustic signals. Presented at *SPIE Defense + Commercial Sensing*, Orlando, Florida, United States, 2018-04-15 - 2018-04-19. (LA-UR-18-23360)

R. Mullin, E. R., S. F. Nowicki, N. A. Debardeleben, S. P. Blanchard, G. W. Mckinney and S. A. Wender. Neutron Scatter Camera Optimization Study for Space Science and National Security Applications. . (LA-UR-19-28392)

Mumpower, M. R., T. M. Sprouse and R. Surman. Nuclear physics for nucleosynthesis: the astrophysical merger of neutron stars. . (LA-UR-20-27832)

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

Nichols, K., S. Dorfman, V. Roytershteyn, B. Van Compernolle, C. Cattle, G. L. Delzanno and B. E. Carlsten. Plasma Waves Generated by Energetic Electrons Injected into Magnetized Plasma at the Large Area Plasma Device at UCLA. Presented at *CSES Presentations*, Los Alamos, New Mexico, United States, 2018-10-09 - 2018-10-09. (LA-UR-18-29722)

Nisbet, H. D., A. Migdissov, A. E. Williams-Jones, V. van Hinsberg and H. Xu. The Solubility of Thorium in Carbonate-Bearing Solutions at Hydrothermal Conditions. Presented at *Goldschmidt Conference (Virtual)*, Los Alamos, New Mexico, United States, 2021-07-04 - 2021-07-09. (LA-UR-21-25841)

Ollila, A. M., S. M. Clegg, A. L. Reyes-Newell and J. M. McGlown. Advancing the readiness level of LunaLIBS for future exploration of the Moon. . (LA-UR-19-28055)

Paris, M. W., G. M. Fuller and L. A. Johns. Quantum Effects on Cosmological Observables as a Probe of BSM & Nuclear Physics. Presented at *CSES Astrophysics Focus Area Symposium*, Los Alamos, New Mexico, United States, 2019-08-15 - 2019-08-15. (LA-UR-19-28224)

Pinilla-Orjuela, M. I., P. F. Bloser, J. R. Tutt, K. E. Mesick, S. F. Nowicki, M. R. Mumpower, C. M. Ticknor, Z. He, Y. Zhu and R. Miller. Lunar CubeSat Mission for High Sensitiivity Nuclear Astrophysics. Presented at *CSES Astrophysics Symposium*, Los Alamos, New Mexico, United States, 2020-10-01 - 2020-10-01. (LA-UR-20-28030)

Rougier, E., E. E. Knight, J. C. Stormont and M. M. Reda Taha. Correlating Damage, Fracture and Permeability in Rocks subjected to High Strain Rate Loading. . (LA-UR-20-28070)

Rougier, E., E. E. Knight and C. R. Bradley. Rock Damage Implications on Permeability Changes. . (LA-UR-18-28934)

Rougier, E., S. H. S. Boyce, Z. Lei, B. J. Euser and E. E. Knight. HOSS A Multi-Physics Toolkit. . (LA-UR-21-22356)

Sibley, A. M. and S. A. Sevanto. Adaptation of juniper and pinon pine to high temperature in the Survival Mortality experiment (SUMO). Presented at *Western Forestry Graduate Research Symposium*, Corvallis, Oregon, United States, 2019-04-26 - 2019-04-26. (LA-UR-19-23809)

Solander, K. C., A. Roy, M. Chen, E. M. Casleton, J. B. Dann, M. D. Wahl, A. A. Tavakoly and C. J. Wilson. Climate variability and fill rate impacts on downstream flows from the Grand Ethiopian Renaissance Dam (GERD). Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32193)

Solander, K. C., A. Roy, M. Chen, E. M. Casleton, M. D. Wahl, A. A. Tavakoly, E. R. Lathrop and C. J. Wilson. Climate variability and fill rate impacts on downstream flows from the Grand Ethiopian Renaissance Dam. . (LA-UR-19-28444)

Sprouse, T. M. Influence of statistical uncertainties of Skyrme-type nuclear mass models on r-process nucleosynthesis simulations. Presented at *FIRE Collaboration*, Upton, New York, United States, 2019-06-11 - 2019-06-12. (LA-UR-19-25443)

Sprouse, T. M., M. R. Mumpower and R. Surman. Portable Routines for Integrated nucleoSynthesis Modeling (PRISM): a flexible nuclear reaction network for astrophysical applications. Presented at *CTA Astrophysics Seminar*, Los Alamos, New Mexico, United States, 2019-08-08 - 2019-08-08. (LA-UR-19-27743)

Sprouse, T. M., M. R. Mumpower and R. Surman. Following fission products in explosive astrophysical environments. Presented at *International Workshop on Fission Product Yields 2019*, Santa Fe, New Mexico, United States, 2019-10-02 - 2019-10-02. (LA-UR-19-30648)

Ulrich, D. E., S. A. Sevanto and J. M. Dunbar. Impacts of soil microbial communities on plant physiological response to drought. Presented at *Ecological Society of America*, New Orleans, Louisiana, United States, 2018-08-06 - 2018-08-09. (LA-UR-18-27243)

Walker, A. C., K. Sakaguchi and S. M. Graf. Analysis of DREAM Reconstructed Fluxes. Presented at *CSES Space Symposium*, Los Alamos, New Mexico, United States, 2020-10-05 - 2020-10-05. (LA-UR-20-27811)

Walker, A. C. and S. K. Morley. DREAM utilizing real-time Van Allen probe data. . (LA-UR-18-29663)

Xu, C., D. W. Goodsman, B. Aukema, N. McDowell, R. Knox, R. Fisher, C. Koven, K. Bleiker and C. Whitehouse. Development of an Insect Outbreak Model for Use in Earth System Models. Presented at *Entomology Society of America*, Denver, Colorado, United States, 2017-11-05 - 2017-11-08. (LA-UR-17-30016)

Yuan, B., Y. J. Tan, M. K. Mudunuru, P. A. Johnson, O. E. Marcillo, A. A. Delorey and S. Karra. Forecasting CO2-driven cold-water geyser eruptions. Presented at *AML Summer School*, Los Alamos, New Mexico, United States, 2018-08-02 - 2018-08-02. (LA-UR-18-27553)

Yuan, F., Y. Li, H. Li, S. Li, L. Ricci, T. Birnstiel, A. Isella, M. Ansdell, J. Drazkowska and S. Stammler. Dust Growth in Protoplanetary Disks and its Observational Implications. Presented at *An informal meeting at Xinjiang Astronomical Observatory*, Urumqi, China, 2019-08-10 - 2019-08-10. (LA-UR-19-28057)

Yuan, F., Y. Li, H. Li, S. Li, R. Luca, T. Birnstiel, A. Isella, M. Ansdell, J. Drazkowska and S. Stammler. Dust Growth in Protoplanetary Disks and its Observational Implications. Presented at *An formal meeting at Xinjiang Astronomical Observatory*, Urumqi, China, 2019-08-10 - 2019-08-10. (LA-UR-19-28058)

Posters

N. Albright, M. B., L. A. Gallegos-Graves, J. C. Thompson, R. Johansen, D. Ulrich, K. L. Avery, B. Timalsina, K. K. Stringfield, A. C. Runde, D. L. Lopez, T. M. Yoshida, M. Shakya, S. A. Sevanto and J. M. Dunbar. Principles for Microbiome Engineering. . (LA-UR-19-28938)

Bloser, P. F., W. T. Vestrand, L. P. Parker, D. C. Poulson, M. I. Pinilla-Orjuela, K. Smith, A. S. Hoover, S. F. Nowicki, A. V. Klimenko and R. M. Kippen. Experimental Gamma-Ray Astronomy at Los Alamos National Laboratory. Presented at *The 36th Annual New Mexico Symposium*, Online, New Mexico, United States, 2020-11-13 - 2020-11-13. (LA-UR-20-29262)

Caldwell, W. K., A. Hunter, C. S. Plesko and S. Wirkus. Impact Crater Models of Asteroids in Forthcoming NASA Missions. Presented at *Lunar and Planetary Science Conference*, The Woodlands, Texas, United States, 2020-03-16 - 2020-03-20. (LA-UR-20-22013)

Caldwell, W. K., A. Hunter and C. S. Plesko. Exploring Porosity in Asteroid 16 Psyche with 3D Hydrocode Modeling of Its Deepest Impact Structure. Presented at *AGU Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-32063)

Conley, J. L., A. Jonko, R. R. Linn and K. Yedinak. A Hot Mess: Seeking Chaos in Marginal Wildland Fire Conditions. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27218)

Doan, H. T., C. Pantea and V. Chillara. Understanding the Acoustic Emissions from Gas Bubble Dynamics A Signature of CO2 Leaks. Presented at *2019 Sandia National Labs Postdoctoral Technical Showcase*, Albuquerque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-32585)

Doan, H. T., V. Chillara and C. Pantea. Understanding the Acoustic Emissions from Gas Bubble Dynamics A Signature of CO2 Leaks. Presented at *APS March 2020 Conference*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21702)

Festal, S., S. Czarnecki, P. J. Gasda, S. F. Nowicki and C. Hardgrove. The sensitivity to boron of the DAN neutron spectrometer on the Mars Curiosity rover. Presented at *Los Alamos Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26606)

Froment, M. Seismic Modeling of Meteorite Impacts on the Surface of Mars.. . (LA-UR-20-25070)

Froment, M., P. Lognonn\xc3\xa9, C. Larmat, Z. Lei, E. Rougier and T. Kawamura. The seismic source of meteorite impacts : a new model combing the seismic representation theorem with numerical simulation.. Presented at *Congress of the PhD students of the STEP'UP doctoral school*, Paris, France, 2021-07-01 - 2021-07-01. (LA-UR-21-25811)

Greess, S. M., A. J. Stanier, J. Egedal, W. S. Daughton, C. B. Forest, J. Olson, A. Y. Le, R. Myers and A. Millet-Ayala. Comparative studies of magnetic reconnection in kinetic simulations and laboratory experiments. Presented at *International Conference on Numerical Simulations of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-29040)

Guardincerri, E., C. A. Rowe, E. S. Schultz-Fellenz, C. Morris, J. D. Bacon, J. M. Durham, D. J. Morley, K. O. Plaud-Ramos, D. C. Poulson, M. Roy, N. George, A. Bonneville and R. Kouzes. 3D Tomography of a Mesa Using Cosmic Ray Muons Detected in an Underground Tunnel. Presented at *AGU Fall Meeting*, San Francisco, California, United States, 2016-12-12 - 2016-12-16. (LA-UR-16-29293)

Guo, F., X. Li, W. S. Daughton, H. Li, Y. Liu and D. D. Ma. New Insights on the Dominant Acceleration Mechanism and Formation of Power-law distribution during Anti-parallel Relativistic Magnetic Reconnection. Presented at *60th annual meeting of the APS division of plasma physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-31750)

Guzik, J. A., J. Jackiewicz, G. Catanzaro and M. S. Soukup. Do Metallic-Line A (Am) Stars Pulsate? Results from TESS Cycles 1-3. Presented at *TESS Science Conference II*, Online,

Massachusetts, United States, 2021-08-02 - 2021-08-06. (LA-UR-21-27101)

Holmes, R. M., C. T. Weaver and D. Palmer. ELROI: A satellite license plate to simplify space object identification. Presented at *AMOS 2018*, Wailea, Hawaii, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28390)

Huang, C., P. Karpov, G. Pilania, C. L. Fryer and S. Woosley. Machine Learning for Turbulence in Supernovae. Presented at *NSF Workshop on Exuberance of Machine Learning in Transport Phenomena*, Dallas, Texas, United States, 2020-02-10 - 2020-02-11. (LA-UR-20-21219)

Jonko, A., K. Yedinak, J. L. Conley, R. Parsons and R. R. Linn. Sensitivity of fire behavior in grassy fuels to small perturbations in the wind field. Presented at *AGU Fall Meeting 2018*, Washington, D.C., District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31459)

Karpov, P., C. Huang, G. Pilania, C. L. Fryer and S. Woosley. Machine Learning for Turbulence in Supernovae. Presented at *234th Meeting of the American Astronomical Society*, St. Louis, Missouri, United States, 2019-06-09 - 2019-06-13. (LA-UR-19-25193)

Karra, S., M. K. Mudunuru and V. V. Vesselinov. A machine learning framework to understand reactive-transport mixing. Presented at *CoDA*, Santa Fe, New Mexico, United States, 2018-03-07 - 2018-03-09. (LA-UR-18-21878)

H. Kilian, P. F., F. Guo, X. Li and H. Li. Detecting the Particle Acceleration Mechanism in Mildly Relativistic Reconnection. Presented at *26th International Conference on Numerical Simulation of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28772)

Kurtakoti, P. K. and C. Veneziani. Great Weddell Sea Polynyas: Mechanisms for their Genesis in a High-Resolution Earth System Model. Presented at *Ocean Sciences Meeting*, Portland, Oregon, United States, 2018-02-11 - 2018-02-16. (LA-UR-18-21166)

Leyba, J., C. Rusch, J. Stormont, M. Reda Taha, E. Rougier, E. E. Knight and B. J. Euser. Modelling the significance of a rubber sleeve on the indirect tensile strength of concrete. Presented at *2nd International Discrete Fracture Network Engineering Conference*, Seattle, Washington, United States, 2018-06-20 - 2018-06-20. (LA-UR-18-25299)

Li, J., A. M. Dempsey, H. Li and S. Li. Ring Formation in Protoplanetary Discs Driven by an Eccentric Instability. Presented at *Distorted Astrophysical Discs: New Insights and Future Directions*, Online, New Mexico, United States, 2021-05-17 - 2021-05-20. (LA-UR-21-24581)

Lin, Y., R. A. Rojas Gomez, J. Yang, J. P. Theiler and B. E. Wohlberg. Data-Driven FWI Methods for Seismic Imaging: Generalization and Robustness Study. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27819)

Lin, Y., Y. Yang, B. Gremillion, X. Zhang and B. E. Wohlberg. SPATIOTEMPORALDATAAUGMENTATION FOR SCIENTIFIC PROBLEMS: AN APPLICATION TO SEISMIC IMAGING. Presented at *The International Conference for High Performance Computing (Virtual Online)*, Los Alamos, New Mexico, United States, 2020-11-09 - 2020-11-09. (LA-UR-20-26420)

Lin, Y. and T. Wang. EarthquakeGen: Earthquake Generator Using Generative Adversarial Networks. Presented at *SEG Annual Meeting*, San Antonio, Texas, United States, 2019-09-16 - 2019-09-16. (LA-UR-19-29447)

Lin, Y. and Y. Wu. InversionNet: Accurate and Efficient Seismic Waveform Inversion with Convolutional Neural Networks. Presented at *AGU*, Washington,, District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31416)

Lundeen, J. A. Searching for Dark Dwarfs With HAWC. Presented at *International School of Cosmic Ray Astrophysics*, Erice, Italy, 2018-08-01 - 2018-08-07. (LA-UR-18-29504)

Mudunuru, M. K., P. A. Johnson, S. Karra, O. E. Marcillo, A. A. Delorey and G. D. J. Guthrie. Extracting eruption dynamics signatures of CO_2-driven cold-water geysers using machine learning. Presented at *CoDA*, Santa Fe, New Mexico, United States, 2018-03-07 - 2018-03-09. (LA-UR-18-21877)

Pinilla-Orjuela, M. I., P. F. Bloser, J. R. Tutt, K. E. Mesick, S. F. Nowicki, M. R. Mumpower and R. Miller. A Lunar CubeSat Mission for High-Sensitivity Nuclear Astrophysics. Presented at *SPIE Astronomical Telescopes and Instrumentation*, Online, New Mexico, United States, 2020-12-14 - 2020-12-18. (LA-UR-20-29828)

Rusch, C., J. Leyba, E. Rougier, E. E. Knight, M. Reda Taha and J. Stormont. Measuring apparent air permeability of concrete during Brazilian tension testing. Presented at *2nd International Discrete Fracture Network Engineering Conference*, Seattle, Washington, United States, 2018-06-20 - 2018-06-20. (LA-UR-18-25289)

Shakya, M., M. B. N. Albright, J. M. Dunbar and P. S. G. Chain. Characterizing Viruses from Soil.. Presented at *Microbiome to Function*, santa fe, New Mexico, United States, 2019-09-15 - 2019-09-17. (LA-UR-19-29063)

Solander, K. C., T. M. Holland, M. D. Hurteau, N. G. McDowell, C. Xu, S. A. Sevanto and R. R. Linn. The expansion of the wildfire season in the western US as seen through FIRETEC. Presented at *American Geophysical Union*, Washington, District Of Columbia, United States, 2018-12-09 - 2018-12-14. (LA-UR-18-31320)

Sprouse, T. M., M. R. Mumpower, R. Navarro Perez, R. Surman, G. McLaughlin and N. Schunck. Implementing and evaluating modern nuclear models in the study of r-process nucleosynthesis. Presented at *2019 Scientific Discovery through Advanced Computing Principal Investigator Meeting*, Rockville, Maryland, United States, 2019-07-16 - 2019-07-18. (LA-UR-19-26508)

Sprouse, T. M., M. R. Mumpower, R. Navarro Perez, R. Surman, G. McLaughlin and N. Schunck. Implementing and evaluating modern nuclear models in the study of r-

process nucleosynthesis. Presented at *Los Alamos National Laboratory Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26744)

Ulrich, D. E., S. A. Sevanto, S. K. Peterson and J. M. Dunbar. The effect of soil microbial communities on variation in physiological responses to drought in loblolly pine (Pinus taeda) seedlings\xc2\xa0. Presented at *American Geophysical Union*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-30965)

Yedinak, K., A. Jonko, R. R. Linn, J. L. Conley, R. Parsons and A. L. Atchley. Chaotic Attractors in Wildland Fire Behavior. Presented at *2018 AGU Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31643)

Other

Caldwell, W. K. Caldwell Portrait. Audio/Visual. (LA-UR-19-22103)

Curtis, S. and J. M. Miller. Broadband Light Curves and Spectra for a Suite of Core-Collapse Supernovae. Dataset. (LA-UR-21-24547)

Larmat, C. Answers to the quiz of Week 3 of InSight at home for teens.. Audio/Visual. (LA-UR-20-23329)

Miller, J. M., J. Lippuner, R. T. Wollaeger, T. M. Sprouse and M. R. Mumpower. Simulations of Neutrino-Driven Accretion Flows. Dataset. (LA-UR-20-29317)

Salvesen, G. M. and J. M. Miller. Black Hole Spin in X-ray Binaries: Giving Uncertainties an f. Dataset. (LA-UR-20-28697)

Vira, A. D., P. A. Fernandes, H. O. I. Funsten, S. K. Morley, H. Yamaguchi, F. Liu and N. A. Moody. Supporting Information for Angular Scattering of Protons through Ultrathin Graphene Foils: Application for Time-of-Flight Instrumentation. Dataset. (LA-UR-19-25024)

Vira, A. D., P. A. Fernandes, R. M. Skoug, H. O. I. Funsten and D. B. Reisenfeld. Supporting Information for Understanding Resolution of Foil-Based Time-of-Flight Mass Spectrometry. Dataset. (LA-UR-19-31581)

Weapons Systems

Identifying Structure-Property Relationships in High Explosives: Using Nitrogen-14 Nuclear Magnetic Resonance (NMR) to Determine Processing Differences and Defect Effects in Materials

Michael Janicke
20210876ER

Project Description

"What is a detonation wave in this microscopic approach and which are the problems to be analyzed in order to define the molecular and crystalline conditions which characterize a molecular crystal as an explosive? In other words, more directly, in order to bring some answer to the question: 'why does an explosive explode' or if you prefer why could it not explode?" This quote taken from a computational paper titled "Fundamental Physics and Chemistry Behind Molecular Crystal Detonations at a Microscopic Level" eloquently outlines many of the challenges facing Los Alamos National Laboratory's (LANL's) chemistry approaches in the field of energetic materials. Detailed knowledge of the atomic and microstructure of nitrogen based mission-relevant materials (i.e. explosives) is fundamental to our understanding them: as they age, as we re-engineer them to replace materials in the stockpile, as they become part of ever evolving accident and threat scenarios. This team is utilizing existing LANL technology and expertise to demonstrate that Nuclear Magnetic Resonance (NMR), the foundation of Magnetic Resonance Imagine (MRI), can safely, quantitatively, and non-destructively characterize materials of high mission relevance and address some of these issues raised above.

An Exploration of the Phase Diagrams and Piezoelectric Properties of High Explosive Crystals at Extreme Conditions

Malcolm Burns
20210943PRD2

Project Description

This work intends to study the phase diagram of the explosive crystal cyclotrimethylenetrinitramine (RDX) with an emphasis on the piezoelectric properties of each phase. RDX is an explosive crystal commonplace in conventional and nuclear weapons, both in the United States stockpile, but also utilized by foreign nations not aligned to US interests. The accurate modeling of explosives is important in both the design and disablement of such weapons. It is imperative that all phenomenon encountered in the detonation of such devices are included in such modeling. To date no effort has included the occurrence of piezoelectricity in phases on the detonation pathway. In this project the piezoelectric nature of the RDX will be explored with the aim to provide experimental data that will underpin Los Alamos National Laboratory's modelling efforts in this field.

Publications

Presentation Slides

Chidester, B. A., M. Harwell, J. Badro, D. Spaulding, M. Huff, P. Kalita, R. Caracas, S. B. Jacobsen and S. Stewart. Shock response of a magma ocean analog to 1 TPa. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2021-12-13 - 2021-12-17. (LA-UR-21-31967)

Enabling Design Agility in a Joint Test Assembly Flight Body (U)

John Minotti
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Project Description

New materials with enhanced properties and behaviors are continually being developed for use in weapons systems. However, there is currently a large disconnect between the fabrication of a new material component and the ability to rapidly assess its benefits in a real-world environment. This is not only due to a lack of collegial research-based interactions between materials scientists with weapons systems engineers, but also from a long, arduous process of specifying requirements and ensuring that any new material meets or exceeds these in their entirety. Put simply, these obstacles have resulted in many new and potentially useful materials sitting "on the shelf" with no clear path to serving the nation in any meaningful way. This project seeks to modernize the manner in which new materials are screened, tested and optimized in flight environments. Here the team will utilize new technologies for polymer cushions and structural mounts as an illustrative example of how process flexibility in materials synthesis techniques can aid in developing a more agile and responsive methodology for evaluating these materials in real-world environments. This work is a collaboration between materials science researchers and the Flight Integration Engineering group at Los Alamos National Laboratory.