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:  
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)
# Table of Contents

## Complex Natural and Engineered Systems

20 Overview

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

58 Directed Plant-Microbiome Evolution for Food and Biofuel Security
- Sanna Sevanto

61 Structured Electrodes for Energy Conversion, Energy Storage, and Ionic Separations
- Jacob Spendelow

65 Model-Driven Data Fusion for Disease Forecasting
- Carrie Manore

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

68 Advanced Characterization to Enable Prediction of Actinide-Molten Salt Behavior
- Marisa Monreal

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

75 Adaptation Science for Complex Natural-Engineered Systems
- Donatella Pasqualini

79 BioManufacturing with Intelligent Adaptive Control: BioManIAC
- Babetta Marrone

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

85 Crucial Radioactive Gas Transport Feedbacks from the Blast Cavity toward the Atmosphere
- Philip Stauffer

86 Passive MemComputing in Lithographic Arrays of Interacting Magnetic Nanoislands
- Francesco Caravelli

88 Reshaping Bacterial Metabolic Output by Deciphering the Determinants of Messenger Ribonucleic Acid (mRNA) Decay
- Christina Steadman

89 The Genetic Patterns of Migration in Global Pandemics
- Andrey Lokhov

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

92 Small Things Considered: Are Viruses as Important to Carbon Cycling in Soils as in Oceans?
- Migun Shakya

93 Engineering green factories for the production of renewable chemicals
- Taraka Dale

94 Inverse Problem Approach to Spacecraft Charging Simulations
- Gian Delzanno

96 Nanotherapeutic Adjuvants for Sepsis
- Jessica Kubicek-Sutherland

98 Particle Modeling of High-Altitude Nuclear Explosions
- Ari Le

100 Capturing the First Uranium Alkylidene Complex
- Jaqueline Kiplinger

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

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

104 Local Transition Modeling for Mixing
- Daniel Israel

105 Grid Scale Energy Storage Using Hydrazine Produced from Lanthanide Electrocatalysis
- Benjamin Davis

106 Blurring the Lines Between Ocean Parameterization and Large Eddy Simulation
- Luke Van Roekel

107 New Possibilities and Discovery Methods for Explosives Synthesis and Formulation
- William Perry
<table>
<thead>
<tr>
<th>Page</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>108</td>
<td>Cold Plasma and Plasmapause Instabilities: A Possible Driver for Long-Lived Drainage Plumes, Giant Undulations and STEVE (Strong Thermal Emission Velocity Enhancement) Aurora</td>
<td>Michael Henderson</td>
</tr>
<tr>
<td>109</td>
<td>Multi-axis Dynamic Modeling of Environmental Capture Re-entry Body Configuration</td>
<td>Matthew Belobrajdic</td>
</tr>
<tr>
<td>110</td>
<td>Terbium-161 for targeted radionuclide therapy</td>
<td>Veronika Mocko</td>
</tr>
<tr>
<td>111</td>
<td>Identifying Viral Variants of Concern in a World of Noisy Evolution</td>
<td>Emma Goldberg</td>
</tr>
<tr>
<td>112</td>
<td>Visualizing and Understanding Complex Fluid Transport in 3-Dimensional Microstructure</td>
<td>Hari Viswanathan</td>
</tr>
<tr>
<td>115</td>
<td>In Situ Characterization of Uranium Hydriding Corrosion</td>
<td>Terry Holesinger</td>
</tr>
<tr>
<td>117</td>
<td>Chemistry of a New Oxidation State for the Early Transuranic Elements</td>
<td>Andrew Gaunt</td>
</tr>
<tr>
<td>119</td>
<td>Understanding and Predicting Hydrocarbon Behaviors in Nanopores of Tight Reservoirs</td>
<td>Qinjun Kang</td>
</tr>
<tr>
<td>122</td>
<td>Using Solar Energetic Protons to Monitor the Outer Magnetosphere</td>
<td>Steven Morley</td>
</tr>
<tr>
<td>124</td>
<td>Innovating Wildfire Representation in Earth System Models (ESMs)</td>
<td>Alexandra Jonko</td>
</tr>
<tr>
<td>126</td>
<td>Illuminating Plutonium: Spectroelectrochemistry in High Temperature Molten Salts</td>
<td>Benjamin Stein</td>
</tr>
<tr>
<td>127</td>
<td>Biogenic Uranium Isotope Fractionation for Biotechnology</td>
<td>Robert Williams</td>
</tr>
<tr>
<td>129</td>
<td>Understanding Glycan Dynamics and Heterogeneity for Effective Human Immunodeficiency Virus (HIV) Vaccine Development</td>
<td>Kshitij Wagh</td>
</tr>
<tr>
<td>131</td>
<td>An Actinium-225/Bismuth-213 Generator Based on Millifluidics Controlled Electrodeposition for Radiopharmaceutical Applications</td>
<td>Michael Fassbender</td>
</tr>
<tr>
<td>132</td>
<td>Next Steps to Molecular Actinide Nitrides</td>
<td>Marisa Monreal</td>
</tr>
<tr>
<td>133</td>
<td>Universal first response countermeasures for current and future pandemic threats: Broad Spectrum Antivirals targeting Host Proteins</td>
<td>Jurgen Schmidt</td>
</tr>
<tr>
<td>134</td>
<td>REECoVER: Recovering Critical Rare Earth Elements (REEs) and Cobalt (Co) from End-of-Life Permanent Magnet Waste</td>
<td>Jaqueline Kiplinger</td>
</tr>
<tr>
<td>135</td>
<td>Electric Field Swing Adsorption - A Process Intensification Tool For Selective Removal of Specific Molecules</td>
<td>John Gordon</td>
</tr>
<tr>
<td>136</td>
<td>Electromagnetic Pulse (EMP) Impacts On Telecommunication Networks</td>
<td>Michael Rivera</td>
</tr>
<tr>
<td>137</td>
<td>Quantification and Modelling of Immune Responses to Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) Infection</td>
<td>Carmen Molina-Paris</td>
</tr>
<tr>
<td>139</td>
<td>Modeling the Transport of Compressible Fluids Through Human Engineered Environments at Scale and their Interactions with Natural Environments</td>
<td>Russell Bent</td>
</tr>
<tr>
<td>140</td>
<td>Carbon Dioxide Conversion to Fuels and Chemical Feedstocks</td>
<td>Piotr Zelenay</td>
</tr>
<tr>
<td>141</td>
<td>Epitope mapping and crystal structures of neutralizing Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV-2) antibodies</td>
<td>Julian Chen</td>
</tr>
<tr>
<td>142</td>
<td>Perovskite Materials for Driving Carbon Dioxide Photo-Reduction</td>
<td>Rajinder Singh</td>
</tr>
<tr>
<td>143</td>
<td>The ecology and evolution of Hantaviridae in the Americas</td>
<td>Ethan Romero-Severson</td>
</tr>
<tr>
<td>144</td>
<td>Drug Discovery by Automated Adaptation of Chemical Structure and Identity</td>
<td>Christopher Neale</td>
</tr>
<tr>
<td>145</td>
<td>Studying Recombination in Ribonucleic Acid Viruses and its Implications for Outbreak Surveillance and Health Interventions</td>
<td>Elena Giorgi</td>
</tr>
<tr>
<td>147</td>
<td>Photochemistry of Actinides in Ionic Liquids for Advanced Separations</td>
<td>Janelle Droessler</td>
</tr>
<tr>
<td>148</td>
<td>Computational and Experimental Bioprospecting of Algae for Antimicrobial Compounds</td>
<td>Blake Hovde</td>
</tr>
</tbody>
</table>
Promoting Carbon Dioxide (CO2) Mineralization During Geologic Carbon Sequestration in Mafic and Ultramafic Rocks
Chelsea Neil

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

A Multiphysics Energy Approach to Modeling the Earth’s Response to Underground Explosions
Kane Bennett

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

Illuminating the Subsurface with Nonlinear Behavior
Andrew Delorey

Molecular Multi-Actinide Cores to Model Surface Reactivity
Aaron Tondreau

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

Investigating Actinide-Based Molecular Magnetism with Electron Paramagnetic Resonance
Benjamin Stein

Multiscale Quantitative Description of Drug Resistance Mechanisms in Bacterial Systems
Sandrasegaram Gnanakaran

Toward a Universal Description for Aqueous Solutions
Alp Findikoglu

Forecasting Valley Fever Disease Risk Using Machine Learning
Carrie Manore

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

Identifying Geometric Constraints Imposed by Antibiotics on Biomolecular Machines
Karissa Sanbonmatsu

Valorization of Lignin for the Production of High Performance Sustainable Aviation Fuels
Cameron Moore

Pore Size and Wettability of Control Electrodes for Next Generation Hydrogen Fuel Cells
Rangachary Mukundan

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

Molecular Basis of Ras-related Cancers
Angel Garcia

Unusual Oxidation States and Covalency-Tuning in Transuranic Molecules
Conrad Goodwin

New First Row Transition Metal Based Catalysts for Sustainable Energy Production
John Gordon

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

Enabling Artificial Selection Programs through Characterizing the Lifecycle of Green Algae
Shawn Starkenburg

Geochemical-Geomechanical Feedback in Stressed Fracture Systems
James Carey

Agile System for Electrochemical Dissolution of Bulk Actinide Oxides
Benjamin Karmiol

Computational Modeling Tool for Rapid Performance Characterization of Novel High-explosive Design Geometries
Von Whitley

Biotechnology for Regional Climate Resilience
Babetta Marrone

Data Driven Accelerated Fuel Qualification for Nuclear Fuels
Tammie Nelson

Global Trends, Resiliency, and Recovery
Sara Del Valle

Mechanistic Studies of Human Disease
Nicolas Hengartner

The Dynamics of Systems Far From Equilibrium
Angel Garcia

Information Science and Technology

Quantum Chemistry using Quantum Computers
Pavel Dub

Prioritizing the Prior: Advanced Inversion Algorithms for Scientific Data Analysis
Brendt Wohlberg

In-Situ Inference: Bringing Advanced Data Science into Exascale Simulations
Earl Lawrence

Uncertainty Quantification for Robust Machine Learning
Diane Oyen
<table>
<thead>
<tr>
<th>Page</th>
<th>Title</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>204</td>
<td>The Optimization of Machine Learning: Imposing Requirements on Artificial Intelligence</td>
<td>Russell Bent</td>
</tr>
<tr>
<td>206</td>
<td>Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems</td>
<td>Benjamin Nebgen</td>
</tr>
<tr>
<td>208</td>
<td>Machine Learning for Realizing Next-Generation Quantum Hardware</td>
<td>Michael Martin</td>
</tr>
<tr>
<td>211</td>
<td>Enabling Predictive Scale-Bridging Simulations through Active Learning</td>
<td>Timothy Germann</td>
</tr>
<tr>
<td>215</td>
<td>Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics</td>
<td>Boian Alexandrov</td>
</tr>
<tr>
<td>221</td>
<td>Machine Learning for Turbulence</td>
<td>Daniel Livescu</td>
</tr>
<tr>
<td>226</td>
<td>Taming Defects in Quantum Computers</td>
<td>Scott Pakin</td>
</tr>
<tr>
<td>233</td>
<td>Quantum Computing with Strontium Nuclear Qubits</td>
<td>Michael Martin</td>
</tr>
<tr>
<td>235</td>
<td>Topological Relation-Based Image Analysis using Graphs</td>
<td>Diane Oyen</td>
</tr>
<tr>
<td>237</td>
<td>Adaptive High-order Finite Element Arbitrary Lagrangian-Eulerian (ALE) Methods for Multi-material Hydrodynamics</td>
<td>Jacob Waltz</td>
</tr>
<tr>
<td>238</td>
<td>Sampling the Unknown: Robust Modeling of Atomic Potentials</td>
<td>Kipton Barros</td>
</tr>
<tr>
<td>240</td>
<td>Unlocking the Power of Tensor Cores with Mixed Precision Algorithms</td>
<td>Anders Niklasson</td>
</tr>
<tr>
<td>241</td>
<td>Dielectric Antenna Array for Pinpoint Data/Energy Targeting</td>
<td>John Singleton</td>
</tr>
<tr>
<td>242</td>
<td>Accelerating Combinatorial Optimization with Noisy Analog Hardware</td>
<td>Carleton Coffrin</td>
</tr>
<tr>
<td>243</td>
<td>Strategies for Topological Quantum Computing with Braiding of Vortices and Skyrmions</td>
<td>Charles Reichhardt</td>
</tr>
<tr>
<td>245</td>
<td>Deep Learning in a Noisy World: Algorithms for Robust Training and Predictive Uncertainty</td>
<td>Sunil Thulasidasan</td>
</tr>
<tr>
<td>246</td>
<td>Unifying Circuit-Model Quantum Computing and Quantum Annealing</td>
<td>Scott Pakin</td>
</tr>
<tr>
<td>247</td>
<td>Resolving the Energy Transfer from a Nuclear Energy Source to the Ground</td>
<td>Esteban Rougier</td>
</tr>
<tr>
<td>248</td>
<td>Mimetic Tensor-Train Algorithms for High-Dimensional Partial Differential Equations (PDEs) without the Curse of Dimensionality</td>
<td>Gianmarco Manzini</td>
</tr>
<tr>
<td>249</td>
<td>Accelerating Parallel Transport Sweeps with Fully Asynchronous Graph Traversal</td>
<td>David Dixon</td>
</tr>
<tr>
<td>250</td>
<td>Monte Carlo Transport Simulations on a Billion-Core Approximate-Computing Platform</td>
<td>Alex Long</td>
</tr>
<tr>
<td>251</td>
<td>Shape Matching of 3-Dimensional Computer-Aided Design (CAD) Models in Automatic Hexahedral Meshing Workflows</td>
<td>Rao Garimella</td>
</tr>
<tr>
<td>252</td>
<td>Effects of Cosmic Ray Neutrons on Modern High Performance Computing (HPC) Components</td>
<td>Nathan Debardeleben</td>
</tr>
<tr>
<td>254</td>
<td>Massively-Parallel Acceleration of the Dynamics of Complex Systems: a Data-Driven Approach</td>
<td>Danny Perez</td>
</tr>
<tr>
<td>255</td>
<td>Objective Flow Topology</td>
<td>Roxana Bujack</td>
</tr>
<tr>
<td>257</td>
<td>Towards Memristor Supremacy with Novel Machine Learning Algorithms</td>
<td>Francesco Caravelli</td>
</tr>
<tr>
<td>260</td>
<td>Stable, Conservative, High-Order Numerical Methods for Direct Numerical Simulations (DNS) in Complex Geometries</td>
<td>Peter Brady</td>
</tr>
<tr>
<td>262</td>
<td>Statistical Learning in Cyberphysical Systems</td>
<td>Nathan Lemons</td>
</tr>
<tr>
<td>264</td>
<td>Impact of Mobility on Coronavirus (Covid-19) Spread</td>
<td>Leticia Cuellar-Hengartner</td>
</tr>
<tr>
<td>265</td>
<td>Limited Information Tomography</td>
<td>Marc Klasky</td>
</tr>
<tr>
<td>266</td>
<td>Closing the Loop: Real-Time Neuromorphic Agents</td>
<td>Garrett Kenyon</td>
</tr>
<tr>
<td>267</td>
<td>Automatic Colormap Improvement in non-Euclidean Spaces</td>
<td>Roxana Bujack</td>
</tr>
<tr>
<td>269</td>
<td>Enhancing Bayesian Multivariate Adaptive Regression Spline Models Using Concepts from Deep Learning</td>
<td>Devin Francom</td>
</tr>
<tr>
<td>270</td>
<td>Differentiable Programming: Bridging the Gap between Numerical Models and Machine Learning Models</td>
<td>Daniel O’Malley</td>
</tr>
</tbody>
</table>
Distributed Algorithms for Large-Scale Ordinary Differential/Partial Differential Equation (ODE/PDE) Constrained Optimization Problems on Graphs
Kaarthik Sundar

Quantum Information-Based Complexity
Yigit Subasi

Accelerated Monte Carlo Algorithms without Detailed Balance
Ying Wai Li

Statistical Learning for Field Theories
Andrey Lokhov

Numerical Methods for Radiation Hydrodynamics Simulations on Current and Future Advanced Parallel Architectures
Jonas Lippuner

Improving Predictions of Complex Systems with Predictive Discrepancy Models and Data Fusion
David Osthus

Optimizing Scientific Codes in the Presence of Extreme Heterogeneity Using Machine Learning
Eun Jung Park

Discrete Optimization Algorithms for Provably Optimal Quantum Circuit Design
Harsha Nagarajan

Emergent Quantum Phenomena with Tensor Networks
Lukasz Cincio

Error Correction and Speed-up of Near-term Quantum Computing Architectures
Patrick Coles

Quantum Simulation of Quantum Field Theories
Rolando Somma

In Situ Quantification of Damage in High Explosives
David Montgomery

Addressing Data Challenges to Improve Prediction Models
Sara Del Valle

Quantum Information with Atoms in Optical Tweezers
Michael Martin

AI-enabled Electron Dynamics at the Device Scale
Benjamin Nebgen

Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches
Youzuo Lin

On-machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication
Wendel Brown

Toward Automated Interpretation of Large, High Resolution Computed Tomography Volumes (U)
Christopher Stull

Launch Vehicle Detection and Tracking System
John Scott

Artificial Intelligence for Sensing
Aric Hagberg

Quantum Algorithm Development for Optimization
Stephan Eidenbenz

Machine Learning Enhanced Modeling
Enrique Batista

Information Science and Technology Institute (ISTI): Foundational Research in Information Science and Technology
James Ahrens

Proximity Effects at Meso-, Nano-, and Atomic Scales: A new Path to Quantum Functionalities
Han Htoon

Control Of Microstructural Instabilities in Composites (COMIC): A Pathway to Realizing Damage Resistant Metals
Laurent Capolungo

Quantum Photonics with Semiconductor Nanocrystals
Victor Klimov

Aging and Metastability of Delta-Phase Plutonium
Jeremy Mitchell

Investigating How Material’s Interfaces and Dislocations Affect Strength (iMIDAS)
Abigail Hunter

Quantum Materials for the Future

Aging and Metastability of Delta-Phase Plutonium
Jeremy Mitchell

Investigating How Material’s Interfaces and Dislocations Affect Strength (iMIDAS)
Abigail Hunter

Uncovering the Role of 5f-electron Magnetism in the Electronic Structure and Equation of State of Plutonium (U)
Neil Harrison

Rational Design of Halide Perovskites for Next Generation Gamma-ray Detection
Sergei Tretiak

Driven Quantum Matter: A Route Towards Novel Phases
Jianxin Zhu

Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials
Blas Uberuaga
334 Accelerated Aging of Crystalline Plutonium Compounds
Justin Cross

335 Direct Plutonium-239 Nuclear Magnetic Resonance: A
Unique Tool for Understanding Plutonium
Eric Bauer

336 Plutonium-239 Nuclear Magnetic Resonance Studies of
Aging and Defects
Filip Ronning

337 Dynamics of Quantum Phase Transitions
Wojciech Zurek

339 Plutonium Elasticity at Extreme Pressures using
Gigahertz Ultrasound in a Diamond Anvil Cell
Blake Sturtevant

340 Predicting the Impact Sensitivity of New Explosives
through Statistical Modeling
Virginia Manner

341 Shedding Light on Quantum Phenomena in Topological
Chiral Crystals
Nicholas Sirica

343 Transition Metal Nitrides for Efficient Nitrogen
Electrocatalysis
Rangachary Mukundan

344 Design Principles for Skyrmions in f-electron Materials
Shizeng Lin

345 Pushing Past the 100 Tesla Threshold: Designing a
High Conductivity/High Strength Metallic Composite
Conductor
John Carpenter

346 Emergent Infrared Localized Surface Plasmon
Resonances in Doped Spinel Metal Oxide
Nanomaterials
Jennifer Hollingsworth

348 Measurement of Dynamic Friction via Kolsky Bar
Benjamin Morrow

349 Defects and Functional Interfaces for Desalination
Jacob Spendelow

350 Synchrotron-based High-Energy Proton Radiography
Matthew Freeman

351 Electrically Pumped Laser Processed from Solution
Victor Klimov

352 Understanding How Exploding Bridge-Wire (EBW)
Detonators Work
Philip Rae

353 High-Efficiency Steam Electrolysis Using Polymer
Electrolyte Membranes
Yu Seung Kim

354 Ultrafast control of material properties through
shallow-core electrons
Pamela Bowlan

355 Unconventional superconductivity in the Nickelates
Mun Chan

356 Hybrid Thermochromic Nanostructures for Radiative
Heat Emergent Functionalities
Wilton Junior de Melo Kort-Kamp

357 Dynamic Catalysis, Advancing Beyond the Sabatier
Principle
Ulises Martinez

358 Predicting and Controlling Interfacial Defects in Soft
Matter
Matthew Lee

359 Manipulating Gas-Phase Chemistry in High Explosive
Thermal Decomposition
Amanda Duque

360 First Measurement of the Scale Anomaly in Dirac
Semimetals
Michael Pettes

361 Self-powered, low cost semiconductors for smart
computation
Wanyi Nie

362 Accurate and Local Forces for Meso-Scale Methods
Ann Wills

363 Supersonic dislocations? A key to unraveling material
strength under extreme conditions.
Daniel Blaschke

364 Using Earth’s Magnetic Field for Battery Diagnostics
Benjamin Davis

365 Ion Beam Synthesis of Layer-Tunable, Transfer-Free
and Chemically Doped Graphene Films on Arbitrary
Substrates
Yongqiang Wang

366 Utilizing Crystalline Sponges to Perform Single Crystal
X-ray Determination on Trace Amounts of Actinium
Compounds
Brian Scott

367 Electronic Structure of Putative Topological Kondo
Insulators
Mun Chan

368 Visualizing Nanoscale Spatio-Temporal Dynamics in
Single Quantum Systems
Peter Goodwin

369 Improved Biologically Friendly Polymer Drag Reducers
From Novel Architectures
Paul Welch

370 Ultrafast X-ray Imaging Using Slow, Visible Cameras
Pamela Bowlan

371 Tuning Functionality via Dimensionality in 4f-Based
Nanowires
Priscila Rosa
<table>
<thead>
<tr>
<th>Page</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>375</td>
<td>Shockwave Metamaterials: Harnessing Structural Hierarchy for Tailorable Dynamic Response</td>
<td>Dana Dattelbaum</td>
</tr>
<tr>
<td>376</td>
<td>Air-Buoyant Vessel</td>
<td>Miles Beaux</td>
</tr>
<tr>
<td>377</td>
<td>Strongly Interacting Polariton Condensates at Room Temperature</td>
<td>Jinkyoung Yoo</td>
</tr>
<tr>
<td>379</td>
<td>Wavelength-Selective, Electrically Driven Single-Photon Sources Operating at Room Temperature</td>
<td>Istvan Robel</td>
</tr>
<tr>
<td>380</td>
<td>Thermally Expandable Microspheres for Plastic-bonded Explosive (PBX) Properties Control</td>
<td>Amanda Duque</td>
</tr>
<tr>
<td>382</td>
<td>Emergent Bogoliubov Fermi Surface in Unconventional Superconductors</td>
<td>Roman Movshovich</td>
</tr>
<tr>
<td>383</td>
<td>Organic Molecular Electrocatalysts for Hydrogen Evolution Reaction</td>
<td>Piotr Zelenay</td>
</tr>
<tr>
<td>384</td>
<td>Magnetization Fluctuation Spectroscopy as a Dynamic Probe of Emergent Magnetic Phases</td>
<td>Scott Crooker</td>
</tr>
<tr>
<td>386</td>
<td>Mixed Conductors for Enhanced Fuel Cell Performance</td>
<td>Yu Seung Kim</td>
</tr>
<tr>
<td>387</td>
<td>Three-dimension (3-D) Printed Hierarchically Porous Heat Pipe Wicks</td>
<td>Matthew Lee</td>
</tr>
<tr>
<td>388</td>
<td>Superdetonation Shaped Charges</td>
<td>Shawn McGrane</td>
</tr>
<tr>
<td>389</td>
<td>Additive Manufacturing of 3-Dimensional and Graded Density Explosive Structures</td>
<td>Dana Dattelbaum</td>
</tr>
<tr>
<td>390</td>
<td>Engineering Nanoionic Memristive Functionality in 3-Dimensional (3D) Oxide Heterostructures</td>
<td>Dmitry Yarotski</td>
</tr>
<tr>
<td>391</td>
<td>Embedded Sensing and Monitoring Techniques for Small Modular Reactors</td>
<td>Timothy Ulrich</td>
</tr>
<tr>
<td>392</td>
<td>Overcoming the Barriers for Growing Device Quality Ultrawide Bandgap Gallium Oxide Semiconductors</td>
<td>Mark Hoffbauer</td>
</tr>
<tr>
<td>393</td>
<td>Adaptive Framework for Enabling Real-time Feedback During Three-dimensional Mesoscale Microstructure Evolution Measurements</td>
<td>Reeju Pokharel</td>
</tr>
<tr>
<td>394</td>
<td>Plutonium Defect Characterization through Mechanical Deformation</td>
<td>Taylor Jacobs</td>
</tr>
<tr>
<td>395</td>
<td>Synthesis of Aluminum Clusters as Next Generation Explosives</td>
<td>Christopher Snyder</td>
</tr>
<tr>
<td>396</td>
<td>The Role of Defects in Mechanical Instabilities of Additively Manufactured Lattice Materials</td>
<td>Rachel Collino</td>
</tr>
<tr>
<td>397</td>
<td>Kick-Starting the Hydrogen Economy with Transition Metal Nitrides</td>
<td>John Watt</td>
</tr>
<tr>
<td>398</td>
<td>Strain-driven Demonstration of Chiral Superconductivity</td>
<td>Sean Thomas</td>
</tr>
<tr>
<td>399</td>
<td>Strong and Ductile: Towards a New Class of High Entropy Alloys with Outstanding and Optimized Properties</td>
<td>Osman El Atwani</td>
</tr>
<tr>
<td>400</td>
<td>Computational Modeling for the Development of Chiral Quantum Systems</td>
<td>Amanda Neukirch</td>
</tr>
<tr>
<td>402</td>
<td>Electronic Transport in Atomically Thin Materials at Far from Mechanical Equilibrium Conditions</td>
<td>Michael Pettes</td>
</tr>
<tr>
<td>404</td>
<td>Nonlinear Photonics of Topological Phase Transitions in the Graphene Family</td>
<td>Wilton Junior de Melo Kort-Kamp</td>
</tr>
<tr>
<td>406</td>
<td>Overcoming the Curse of Dimensionality to Predict Chemical Reactivity</td>
<td>Beth Lindquist</td>
</tr>
<tr>
<td>408</td>
<td>Novel X-ray Imaging to Unlock the Potential of Antiferromagnetic Materials</td>
<td>Adra Carr</td>
</tr>
<tr>
<td>409</td>
<td>Synthesis of Platinum-Rare Earth Intermetallic Fuel Cell Catalysts</td>
<td>Jacob Spendelow</td>
</tr>
<tr>
<td>410</td>
<td>Designing New Ferroelectric Materials with Spin Crossover Transitions</td>
<td>Wanyi Nie</td>
</tr>
<tr>
<td>411</td>
<td>The Optoelectronic Device Applications of 2-Dimensional Interlayer Moiré Excitons</td>
<td>Han Htoon</td>
</tr>
<tr>
<td>412</td>
<td>Defect tolerant scintillators: Linking structure and performance via machine learning (ML)</td>
<td>Anjana Talapatra</td>
</tr>
<tr>
<td>413</td>
<td>Development of Next Generation Microstructure-aware Burn Models for High Explosives.</td>
<td>Tariq Aslam</td>
</tr>
</tbody>
</table>
Importance of Metal/Oxide Interfaces to Design and Tailor Composite Material Properties. 
Blas Uberuaga

Strain Susceptibility of Quantum Critical Fluctuations
Johanna Palmstrom

Electrically Pumped Laser Diodes Using Charged Colloidal Quantum Dots
Victor Klimov

Design and Discovery of Novel, Two-Dimensional f-electron Quantum Materials
Eric Bauer

Atomistic Modeling and Machine Learning for Bio-advantaged Polymer Design
Ghanshyam Pilania

Highly Ordered Refractory Intermetallics: the ZIA-Phases Project
Stuart Maloy

Design and Discovery of Novel High-entropy Alloys
Saryu Fensin

Topological Superconductivity in Van Der Waals Materials as a Platform for Qubits
Christopher Lane

Synthesis and Stabilization of 2D Electrenes as Novel Nanoscale Magnets
Sergei Ivanov

Multi-scale Visualization for Tuning High-efficiency and Low-catalyst-loading
Ulises Martinez

Characterizing the Spatial and Temporal Evolution of Nuclear Materials during Coupled Irradiation and Corrosion
Nan Li

Ultrafast Spectroscopy of Hybrid Quantum-plasmonic Nanoscale Optical Systems
Houtong Chen

Emergent Phenomena in Magnetically Frustrated f-electron Quantum Materials
Priscila Rosa

Programmable Waveguides of Spin-Polarized Current with "Twisted" Moire Crystals
Scott Crooker

High-performance Photo-sensor/detector by Multiplexed Heterojunction of 2-Dimensional Epitaxial Layers/perovskites/plasmonic Nanoparticles
Aiping Chen

Electrocatalysts for Entirely Platinum Group Metal-free Water Electrolyzer
Piotr Zelenay

In Operando Study of Resistive-switching Devices at Nanoscale
Aiping Chen

Conformal Field Theories with the Bootstrap
Anna Hayes-Sterbenz

Exploration of New Topological States of Matter in Strongly Correlated Materials and in Ultra-high Magnetic Fields
Neil Harrison

Development of an Innovative Mechanical Testing System and Techniques for Characterizing Irradiated Advanced Cladding Concepts and Novel Materials
Jonathan Gigax

Ferromagnetism and Spin Fluctuations in the Atomically-Thin Limit
Scott Crooker

In Situ Mesoscale Response under Combined Pressure-Shear Dynamic Loading
Cynthia Bolme

Ex Machina Hamiltonians for Next-Generation Molecular Simulations
Galen Craven

Exploration of Colossal Thermoelectric Power in 4-fundamental (4f) and 5f Topological Magnets
Filip Ronning

Electrically Driven Optoelectronic Plasmonic Nanodevice in Carbon Nanotubes
Andrew Jones

Unconventional Topological Excitations in Correlated Materials
Nikolai Sinitsyn

Rust, Dust, and a Passive Future - Resilient Actinide Materials (U)
Samantha Lawrence

Solution fabricated solid-state X-ray imager
Wanyi Nie

Modern Radiation Case Material for an Agile Complex
Kendall Hollis

High -Performance/-Precision/-Z (HPPZ) Scintillator Grids via Advanced Electrochemistry
Enkeleda Dervishi-Whetham

Modernizing Detonator Production and Inspection: Robotics meets Additive and Digital Manufacturing
Alexandria Marchi

Integrating Additive Manufacturing and Investment Casting for Complex Metal Architectures with Predictable Mechanics (U)
Matthew Lee
450 Special Carbide for Weapon Applications (U)  
David Jablonski

451 The Use of Additive Manufacturing of High Explosives and its Application to Weapon Safety (U)  
Von Whitley

452 Prompt, Photogated Negative Hydrogen Source  
Rodney Mccrady

453 Understanding Homogenization Kinetics of As-Cast Plutonium Alloys to Improve Manufacturing of Weapons Components (U)  
Jeremy Mitchell

454 In-Situ Ultrasound Grain Refinement in Electron Beam Additive Manufacturing for Improvement of High Strain-Rate Properties (U)  
Cristian Pantea

455 Study for Alternative Cavity Wall and Inductive Insert Material  
Charles Taylor

456 A Novel Heater Wire to Improve H- Ion Source Filament Lifetime  
Prabir Roy

457 Design for Manufacture Pit Feasibility Study (U)  
Christina Scovel

458 Casting: Design Responsiveness and Rapid Qualification  
Kara Luitjohan

459 Welding: Design Responsiveness and Rapid Qualification  
Lindsay O'Brien

460 Powder Materials: Design Responsiveness and Rapid Qualification (U)  
Kendall Hollis

461 The Effect of Defects on the Plutonium Gallium (PuGa) Phase Boundaries (U)  
Donald Brown

462 New Technique for Uranium Hydride Analysis using Ultracold Neutrons  
Zhaowen Tang

463 An Investigation of Variables Affecting Plutonium Hydriding (U)  
Troy Holland

464 Novel in situ Probes of Mesoscale Materials Dynamics  
Dmitry Yarotski

467 Expedited High Explosive Formulation Through Processing-structure-property-performance Relationships  
Kyle Ramos

469 Investigation of the Role of Actinides on the Local Structure of Molten Salts Using Neutron Pair-distribution Function Analysis  
Sven Vogel

470 Accelerated Development of Additively Manufactured Uranium Oxide (UO2) Fuels for Geometries Avoiding Fuel Lifetime-limiting Irradiation Swelling Using Bulk Neutron Characterization  
Bjorn Clausen

471 Molecular Framework Architectures for Quantum Information  
Jennifer Hollingsworth

472 Enhancing Resonant Ultrasound Spectroscopy (RUS) to Measure the Elastic Properties of Complex Multi-Material Actinide Systems for In-Situ Applications  
Timothy Ulrich

473 Method for Extending the Plutonium-238 Supply  
Kirk Weisbrod

474 Rapid Actinide Identification via Luminescence (RAIL) Sensor  
John Ahern

475 Influence of Defects on the alpha to beta Phase Transformation in Plutonium  
Sarah Hernandez

476 Corrosion Protection of Plutonium using Atomic Armor  
Doinita Neiner

477 Seaborg Institute: Center for Advancing Actinide Science and Technology at Los Alamos National Laboratory  
Franz Freibert

479 Theory and Computation on Quantum Systems  
Angel Garcia

485 Theoretical and Experimental Materials Science  
Filip Ronning

Nuclear and Particle Futures

490 The Neutron Electric Dipole Moment as a Gateway to New Physics  
Takeyasu Ito

494 Convincing Search for Sterile Neutrinos at Lujan  
Richard Van De Water

497 A New Era of Nuclear Physics at the Electron-Ion Collider  
Ivan Vitev

502 High-Gradient, High-Efficiency Radio-frequency (RF) Structures: Smart Design Based on Informed Breakdown Suppression  
Evgenya Simakov
Novel Seeding Method for Compact Terahertz (THz) Free Electron Lasers
MD Zuboraj

Production of Shaped Electron Bunches with Diamond Field Emitter Array Cathodes
Evgenya Simakov

Pinning Down the Neutrino-proton Process Importance in Heavy Element Production via Reaction Studies on Radioactive Nickel-56
Hye Young Lee

Ultra-Diffuse Galaxies, Tidal Streams and Dwarf Galaxies: The Low-Surface Brightness Frontier
W Vestrand

Using Quarkonia to Probe Matter from the Early Universe
Ivan Vitev

A New Computation Framework for the Nonlinear Beam Dynamics with Radiation Self-fields
Chengkun Huang

The Influence of Multiple Scattering on the Opacities of Warm and Hot Dense Matter
Charles Starrett

A Non-Invasive Current Profile Diagnostic for Electron Bunches
Quinn Marksteiner

Origin of High-Energy Astrophysical Neutrinos: Multi-messenger Signals from Flares of Extragalactic Jets
Hui Li

Atomic Magnetometry for the neutron Electric Dipole Moment (nEDM) Experiment (Rosen Scholar)
Michael Furlanetto

Advanced Fusion Concept for National Security Applications (U)
William Daughton

An Alternative Approach to Inertial Confinement Fusion (ICF) Ignition and Burn Propagation at the National Ignition Facility (NIF)
Richard Olson

Neutron Experiment in Moon Orbit Pathfinder (NEMO 'Finder)
David Palmer

Probabilistic Uncertainty Quantification Tools for Neutron Analysis
George McKenzie

Measuring and Modeling Void Collapse for Materials Science and Dense Plasma Regimes at the Linac Coherent Light Source
David Montgomery

Actinide Composition of Molten Salt Reactor Fuel from Fission Gases
Anna Hayes-Sterbenz

A Neural Network Framework for Kernel Density Estimator Reconstruction
Mathew Cleveland

A Neutron Target at the Los Alamos Neutron Science Center
Michael Furlanetto

Prediction Improvements of Transient Behavior in Advanced Reactors (PITBAR)
Holly Trellue

Extending High Altitude Water Cherenkov (HAWC) Science to the High and Low Energies
James Harding

Resolving Transport Processes in Multispecies Plasma Shock Waves
Samuel Langendorff

Exploring Inside the Los Alamos Neutron Science Center (LANSCE) Hydrogen- Ion Source with Laser Absorption Techniques
David Kleinjan

Quantum Chromodynamics (QCD) Fragmentation Scaling Laws from Space-Time Reciprocity
Duff Neill

Kinetic Study of a Magnetic-Mirror Wet-Wood-Burner Fusion Neutron Source
Ari Le

Shocked Variable-Density Turbulence
Tiffany Desjardins

Diagnosing Plasma Viscosity in Compressible High-Energy-Density Systems
Joshua Sauppe

MEGAgram (Measurements of Ejecta in GAs): Digital Holography for Ejecta in Extreme Conditions
Dana Duke

Searches for Exotic Spin-dependent Interactions using a Spin-Exchange Relaxation-Free Magnetometer and a Rare-earth Iron Garnet Mass
Pinghan Chu

Adaptive Process Control for Beyond-State-of-the-Art Alkali Antimonide Photocathodes
Vitaly Pavlenko

A Dual n-gamma Detector Array to Correct Neutron Transport Simulations
Keegan Kelly
607  Conservative Slow-Manifold Integrators  
Joshua Burby

609  State-of-the-Art Predictions for the Matter-Antimatter Asymmetry  
Christopher Lee

611  Searching for Dark Matter with Fixed Target Experiments  
Daniele Spier Moreira Alves

612  A Study of Diffusion Around Pulsar Wind Nebulae  
Kelly Malone

614  Towards Data Science Driven Multi-physics Modeling to Probe Neutron Star Mergers  
Jonah Miller

615  Decipher the Coupled Plasma and Atomic Physics for Reactor Plasma Exhaust  
Xianzhu Tang

616  The Urge to Merge: The Fate of Binary Black Holes  
Hui Li

617  Searching for New Physics at the Intensity Frontier at the EIC  
Christopher Lee

619  Next Generation Simulations of the Remarkable Deaths of Massive Stars  
Joshua Dolence

620  Supermassive Black Holes and Their Environment  
Jarrett Johnson

621  Mega Electron Volt (MeV) Gamma-Ray Astronomy: Exploring the Universe in the Nuclear Transition Region  
Lucas Parker

623  Matter and Nuclei at Neutron-Rich Extremes  
Ingo Tews

625  Phase Diagrams and Conductivity in the Interiors of White Dwarf Stars  
Didier Saumon

627  The Ultimate Search for the Color Glass Condensate  
Renaud Boulware

628  Precision Nuclear Tomography at the Electron-Ion Collider  
Ivan Vitev

629  Implementing a Novel Ultrasonic Filtration Technology to Eliminate Hydroxide Precipitation Bottlenecks at TA-55  
James Coons

630  Megavolt generator for multiple-pulse hydrotesting  
Nicola Winch

631  Modeling Late-Time Electromagnetic Pulse and Its Disturbed Atmospheric Environment  
Christopher Jeffery

632  Detector Response Toolkit for Nuclear Emergency Response  
Madison Andrews

633  Nuclear Material Control and Accounting (NMC&A)/In-line Monitoring Capability (ILM)  
Rollin Lakis

634  Demonstration of Advanced Experimental and Theoretical Characterization of Hydrogen Dynamics and Associated Behavior in Advanced Reactors  
Holly Trellue

636  Cryogenically Cooled Particle Accelerators for Transformative Improvement  
Tsuyoshi Tajima

Science of Signatures

638  Hyperspectral Xray Imaging (HXI): Nanochemical Analysis of Actinide and Explosive Materials (U)  
Mark Croce

640  Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter (U)  
Manvendra Dubey

644  Capturing the Origin and Evolution of Persistence Using Real-time, In vivo, Single Cell Transcriptomics  
Murray Wolinsky

646  The Mini Astrophysical Mega Electron-volt Background Observatory (MAMBO) CubeSat Mission: Demonstrating Agile Satellite Platforms for Astrophysics and National Security  
Peter Bloser

648  HEROS - Human Exposure of Radiation using Organ Systems  
Jennifer Harris

649  Basic Science of Underground Nuclear Explosions: Emplacement Condition Signature Discovery  
Thomas Rahn

650  Atomtronics: A New Approach to Sensing, Signal Processing, and Signal Analysis  
Malcolm Boshier

652  Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces  
Abul Azad

656  A Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) Future (U)  
Scott Twary

658  The Remote Elemental, Molecular, and Isotopic Camera (REMICam)  
Samuel Clegg

16
Early Detection of Explosive Volcanic Eruptions Using Very High Frequency (VHF) Radiation from Vent Discharges
Sonja Behnke

Unveiling the Heating and Acceleration of Solar Wind by “Touching” the Sun with the Parker Solar Probe
John Steinberg

Deep Learning Interferometric Synthetic-Aperture Radar
Bertrand Rouet-Leduc

The Role of Defects in Solid State Detonation Kinetics
Pamela Bowlan

Parallel Magnetic Resonance Imaging with a Multichannel Radio-frequency Atomic Magnetometer
Young Jin Kim

Broadband Terahertz Circular Dichroism Spectroscopy
Houtong Chen

A New Approach to Predict Toxicity of Small Molecule Toxins
Hau Nguyen

Long-lived Fauna as Tracers of Anthropogenic Radionuclides
Cyler Conrad

Identification of Gamma Radiation Enabled by Semiconductive Nanocrystalline Materials
Amanda Graff

Most Sensitive Optical Quantum Sensor
Young Jin Kim

Atom Interferometry without Coherence
Malcolm Boshier

Gleaming the Cube: Advanced Focal Planes for Optimal Acquisition of Spectral Images
John Bowlan

Whispering-Gallery-Resonator Beads for Rapid and Sensitive Chemical Threat Detection
Laura Lilley

Dark Field Proton Radiography
Matthew Freeman

Listening for Rock Coatings on Mars: Using Acoustic Signals from Laser-Induced Breakdown Spectroscopy
Nina Lanza

High Dynamic Range Neutron Detector for Pulsed Applications
Markus Hehlen

Using Laser Synthetic Aperture Radar to Image a Low Earth Orbit Satellite
David Thompson

A Low Power Electron Injector for Space Applications
Michael Holloway

Uranium hexafluoride enrichment verification using ultra-low field nuclear magnetic resonance
Per Magnelind

Fission-Acoustic Signature Discovery
Rollin Lakis

Rapid Bioremediation and Simultaneous Enrichment of Uranium by Common Green Algae
Laura Lilley

Imaging Neural Dynamics With Ultra-Low Field Magnetic Resonance Imaging (MRI)
Per Magnelind

Proton Radiography for Advanced Cancer Therapy
Michelle Espy

OrganiCam: A High-Sensitivity Radiation-Hardened Imaging Organic Detector For Space and Programmatic Applications
Roger Wiens

Boron and Ribose in Clay: a Precursor for Life on Earth and Mars?
Patrick Gasda

Reduced-profile Current-sheet Array (CSA) Antenna with Simpler Drive and Better Antenna Efficiency
MD Zuboraj

Quantum Metrology with an Atom Superconducting Quantum Interference Device (SQUID)
Changhyun Ryu

Novel, Fast Enhancements to Bragg Ptychography
Kevin Mertes

Viral Mosaic Biosensor
Jessica Kubicek-Sutherland

Emulating Quantum Magnetism with Rydberg Atoms
Michael Martin

Discovering the 3D Structure and Dynamics of the Sun-Interstellar Medium System on a Global Scale
Daniel Reisenfeld

Rare Earth Fission Product Element Separations by High Speed Counter-Current Chromatography
Iain May

Gossamer Radio Frequency (RF) Satellite Parabola Made by Additive Manufacturing
Jeremiah Rushton

Multi-Int Signature Collection and Exploitation for Security
Dale Anderson

Toward Discovering the Structure and Dynamics of the Sun-Interstellar Medium System
Daniel Reisenfeld
First Nuclear Quadrupole Resonance Observations of an Insensitive High Explosive
Michael Malone

Active Electromagnetic Cloaking for Enhanced Science of Signatures
Abul Azad

Data-Driven Specification of Earth's Magnetic Field
Humberto Godinez Vazquez

Granddaughter Radiochronometry for Nuclear Forensics
Joanna Denton

Using Thundercloud Illumination by Lightning to Understand Optical Signal Propagation in Nature
Michael Peterson

Understanding Optical Signatures from Natural and Artificial Aurora
Rebecca Sandoval

Nitrogen: Abundant on Earth and Forgotten in Space
Philip Fernandes

A High-throughput (RapidPhage) Platform for the Discovery of Lytic Bacteriophages Against Multi-drug Resistance Pathogens
Anand Kumar

Locating Nature's Most Extreme Explosions in Real-time
Lucas Parker

High Efficiency Active Environmental Sampling of Chemical Traces
Ann Junghans

Understanding the Wave Mechanics of Micro-architected Waveguides to Design Acoustic Quick Response Codes
Vamshi Chillara

In-Process, Full Part Defect Detection for Additive Manufacturing
Adam Wachtor

New Innovations in Microtesla Nuclear Magnetic Resonance Spectroscopy
Derrick Kaseman

Improving Public Health by Linking Virus Genetic Evolution and Epidemic Spread
Arshan Nasir

Disease Outcome Analysis for Improved Disease Interventions
Paul Fenimore

Smart Mobile Sensor Platform Development for Radiological Mapping of Large-Scale Areas
Tony Shin

The Seismic Noise is the Signal: Applying Machine Learning to Earthquake Forecasting
Christopher Johnson

The Next Generation of Aerosol Optical Models: Humidity Dependence and Chemical Processing
Manvendra Dubey

Superradiant RNA for Single Molecule In-Vivo Fluorescence Microscopy
Murray Wolinsky

Distinguishing Uranium Oxides using Table-top Extreme Ultraviolet Absorption Spectroscopy to Elucidate Reaction Kinetics and Conglomeration in Uranium-containing Laser Ablation Plasmas
Pamela Bowlan

How Biological Communities Can Unlock Hidden Signatures of Environmental Change
Jeanne Fair

An Atomtronic Rotation Sensor
Malcolm Boshier

Biophysical Interactions of Amphiphiles with Biomimetically Patterned Membranes
Loreen Stromberg

Development and Implementation of a Portable Microfluidic J-Coupled Spectrometer for Rapid Detection and Identification of Emerging Chemical Threats
Derrick Kaseman

Unraveling Lipoprotein Signatures for Tick-Borne Pathogens
Harshini Mukundan

Neutron Spectroscopy for Nuclear Emergency Response Applications
Theresa Cutler

Modeling an Artificial Radiation Belt of Ionized Fission Fragments After a High-altitude Nuclear Explosion (HANE)
Misa Cowee

How Can the Granular Defects of Additive Manufacturing be Evaluated?
Carly Donahue

Exploring Safeguard Signatures with Energy Resolved Neutron Imaging for Future Molten Salt Reactor Designs
Alexander Long

Learning Fault Physics and Failure in Hydraulic Injection
Paul Johnson

Intelligent Coupling of X-ray Radiography and Acoustics for Accurate Rapid Assessments for Emergency Response
John Greenhall
741  Flight Software Framework for Agile Response to Global Security Threats
     Markus Hehlen

742  Advanced Signatures, Processing, and Exploitation for Counter-proliferation (ASPEC)
     Kevin Mitchell

743  Artificial Intelligence (AI)-Driven Collection and Models for Trust/Reliability of Integrated Space Surveillance Data
     W Vestrand

744  Scalable digital biosurveillance to advance pandemic science and preparedness
     Patrick Chain

745  Center for Space and Earth Science (CSES): Foundational Research in Space and Earth Science
     Lisa Danielson

749  Emerging Challenges in Space and Earth Science
     Lisa Danielson

Weapons Systems

764  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

765  An Exploration of the Phase Diagrams and Piezoelectric Properties of High Explosive Crystals at Extreme Conditions
     Malcolm Burns

766  Enabling Design Agility in a Joint Test Assembly Flight Body (U)
     John Minotti
Table of Contents

I. Leadership Perspectives

II. Program Description
   a. LDRD Directives, Objectives, and Strategic Challenges
   b. LDRD Program Values
   c. LDRD Aligns with Laboratory Strategy
   d. Program Structure
      i. Overview
      ii. Director’s Initiatives
      iii. Directed Research
      iv. Exploratory Research
      v. Mission Foundations Research
      vi. Centers Research
      vii. Postdoctoral Research and Development
      viii. Early Career Research
      ix. Reserve/Special Calls
   e. LDRD Objectives Across the Portfolio

III. Program Value
   a. At-a-glance
   b. Mission Relevance
   c. Project Appraisals
   d. Performance Indicators: LDRD at LANL
      i. Intellectual Property
      ii. Peer-reviewed Publications
      iii. Broad Intellectual Engagement
      iv. Science and Engineering Talent Pipeline
      v. The Long-Term Impacts of LDRD Investments

IV. Program Accomplishments
   a. Science in the News
   b. Research Highlights
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.

Leadership Perspectives
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 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
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
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.
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

As of FY21 close.
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**
  - 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**
  - 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 science 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.
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)

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

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

### Weapons Production: Agile and Efficient Nuclear Manufacturing

<table>
<thead>
<tr>
<th>Project Description</th>
<th>Responsible Party</th>
</tr>
</thead>
<tbody>
<tr>
<td>*Implementing a Novel Ultrasonic Filtration Technology to Eliminate Hydroxide Precipitation Bottlenecks at TA-55</td>
<td>James Coons (C-CDE)</td>
</tr>
<tr>
<td>*Agile System for Electrochemical Dissolution of Bulk Actinide Oxides</td>
<td>Benjamin Karmiol (AMPP-4)</td>
</tr>
<tr>
<td>*On-machine Probe Measurement and Compensated Cutting For Improved Plutonium Shell Fabrication</td>
<td>Wendel Brown (PT-2)</td>
</tr>
</tbody>
</table>

### Energy Security: machine learning and molten salt reactors

<table>
<thead>
<tr>
<th>Project Description</th>
<th>Responsible Party</th>
</tr>
</thead>
<tbody>
<tr>
<td>*Inferring the Unobservable with Generalizable, Rigorous, and Domain-Aware Machine Learning Approaches</td>
<td>Youzuo Lin (EES-17)</td>
</tr>
<tr>
<td>Learning Fault Physics and Failure in Hydraulic Injection</td>
<td>Paul Johnson (EES-17)</td>
</tr>
</tbody>
</table>

### Weapons Engineering: Nuclear explosive package

<table>
<thead>
<tr>
<th>Project Description</th>
<th>Responsible Party</th>
</tr>
</thead>
<tbody>
<tr>
<td>*Modern Radiation Case Material for an Agile Complex</td>
<td>Kendall Hollis (SIGMA-1)</td>
</tr>
<tr>
<td>*Megavolt generator for multiple-pulse hydrotesting</td>
<td>Nicola Winch (NEN-2)</td>
</tr>
<tr>
<td>*Computational Modeling Tool for Rapid Performance Characterization of Novel High-explosive Design Geometries</td>
<td>Von Whitley (XTD-SS)</td>
</tr>
</tbody>
</table>

### Global Security: Nuclear emergency response

<table>
<thead>
<tr>
<th>Project Description</th>
<th>Responsible Party</th>
</tr>
</thead>
<tbody>
<tr>
<td>*Neutron Spectroscopy for NER Applications</td>
<td>Theresa Cutler (NEN-2)</td>
</tr>
<tr>
<td>Intelligent Coupling of X-ray Radiography and Acoustics for Accurate Rapid Assessments for Emergency Response</td>
<td>John Greenhall (MPA-11)</td>
</tr>
<tr>
<td>Detector Response Toolkit for Nuclear Emergency Response</td>
<td>Madison Andrews (XCP-7)</td>
</tr>
</tbody>
</table>

*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.)
Reserve/Special Calls

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:

<table>
<thead>
<tr>
<th>Component</th>
<th>Set aside</th>
<th># of projects</th>
</tr>
</thead>
<tbody>
<tr>
<td>DR full project continuations post feasibility review</td>
<td>$1.86 M</td>
<td>2</td>
</tr>
<tr>
<td>ER Seedling new starts</td>
<td>$0.75 M</td>
<td>10</td>
</tr>
<tr>
<td>Early Career new starts</td>
<td>$2.20 M</td>
<td>18</td>
</tr>
<tr>
<td>Mission Foundations Phase 2 continuations</td>
<td>$0.91 M</td>
<td>10</td>
</tr>
<tr>
<td>Director’s Initiative new starts</td>
<td>$4.00 M</td>
<td>TBD</td>
</tr>
<tr>
<td>Postdoc project new starts</td>
<td>$2.65 M</td>
<td>TBD</td>
</tr>
</tbody>
</table>

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 reserve FY22

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.

### Relative Weights of LDRD Objectives During Selection by Component

*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.*
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**

<table>
<thead>
<tr>
<th>Total Program Cost</th>
<th>Total Number LDRD Projects</th>
<th>New LDRD Projects in 2021</th>
</tr>
</thead>
<tbody>
<tr>
<td>$160M</td>
<td>459</td>
<td>201</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LDRD-supported Postdocs</th>
<th>59%</th>
<th>391 of 665 postdocs at Los Alamos</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDRD-supported Postdoc to Staff Conversions</td>
<td>54%</td>
<td>44 of 81 conversions at Los Alamos</td>
</tr>
<tr>
<td>Peer-reviewed Publications</td>
<td>38%</td>
<td>830 of 2,207 publications at Los Alamos</td>
</tr>
<tr>
<td>U.S. Patents Issued</td>
<td>30%</td>
<td>14 of 46 patents at Los Alamos</td>
</tr>
<tr>
<td>R&amp;D 100 Awards</td>
<td>57%</td>
<td>4 of 7 R&amp;D 100 awards at Los Alamos</td>
</tr>
</tbody>
</table>

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.
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.

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

<table>
<thead>
<tr>
<th></th>
<th>FY17</th>
<th>FY18</th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
</tr>
</thead>
<tbody>
<tr>
<td>LANL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>U.S.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>patents</td>
<td>43</td>
<td>51</td>
<td>53</td>
<td>46</td>
<td>46</td>
</tr>
<tr>
<td>LDRD supported</td>
<td>9</td>
<td>10</td>
<td>20</td>
<td>19</td>
<td>14</td>
</tr>
<tr>
<td>% due to LDRD</td>
<td>21%</td>
<td>20%</td>
<td>38%</td>
<td>41%</td>
<td>30%</td>
</tr>
</tbody>
</table>

**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

<table>
<thead>
<tr>
<th></th>
<th>FY17</th>
<th>FY18</th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
</tr>
</thead>
<tbody>
<tr>
<td>LANL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>software copyrights</td>
<td>148</td>
<td>113</td>
<td>147</td>
<td>119</td>
<td>120</td>
</tr>
<tr>
<td>LDRD supported</td>
<td>21</td>
<td>19</td>
<td>16</td>
<td>39</td>
<td>48</td>
</tr>
<tr>
<td>% due to LDRD</td>
<td>14%</td>
<td>17%</td>
<td>11%</td>
<td>33%</td>
<td>40%</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th></th>
<th>FY17</th>
<th>FY18</th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
</tr>
</thead>
<tbody>
<tr>
<td>LANL disclosures</td>
<td>117</td>
<td>109</td>
<td>118</td>
<td>115</td>
<td>101</td>
</tr>
<tr>
<td>LDRD supported</td>
<td>24</td>
<td>40</td>
<td>39</td>
<td>34</td>
<td>33</td>
</tr>
<tr>
<td>% due to LDRD</td>
<td>21%</td>
<td>37%</td>
<td>33%</td>
<td>30%</td>
<td>33%</td>
</tr>
</tbody>
</table>

“Tech Snapshots” on many of these technologies can be found on the Richard P. Feynman Center for Innovation [website](#).
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

<table>
<thead>
<tr>
<th>LDRD supported</th>
<th>FY17</th>
<th>FY18</th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
</tr>
</thead>
<tbody>
<tr>
<td>LANL publications</td>
<td>2,001*</td>
<td>2,100</td>
<td>2,066</td>
<td>1,971</td>
<td>2,207</td>
</tr>
<tr>
<td>LDRD supported</td>
<td>525*</td>
<td>613</td>
<td>714</td>
<td>678</td>
<td>830</td>
</tr>
<tr>
<td>% due to LDRD</td>
<td>26%</td>
<td>29%</td>
<td>35%</td>
<td>34%</td>
<td>38%</td>
</tr>
</tbody>
</table>

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

### Citations

Number of citations of peer-reviewed publications

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

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.)*

![Map showing recent LDRD external collaborators within the United States](image-url)
Science and Engineering Talent Pipeline

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

<table>
<thead>
<tr>
<th></th>
<th>FY17</th>
<th>FY18</th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
</tr>
</thead>
<tbody>
<tr>
<td>LANL Postdocs</td>
<td>497</td>
<td>556</td>
<td>632</td>
<td>655</td>
<td>665</td>
</tr>
<tr>
<td>LDRD supported &gt;10%</td>
<td>263</td>
<td>281</td>
<td>376</td>
<td>363</td>
<td>391</td>
</tr>
<tr>
<td>% due to LDRD</td>
<td>53%</td>
<td>51%</td>
<td>59%</td>
<td>55%</td>
<td>59%</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th></th>
<th>FY17</th>
<th>FY18</th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
</tr>
</thead>
<tbody>
<tr>
<td>LANL Conversions</td>
<td>69</td>
<td>81</td>
<td>87</td>
<td>75</td>
<td>81</td>
</tr>
<tr>
<td>LDRD supported &gt;10%</td>
<td>37</td>
<td>37</td>
<td>39</td>
<td>35</td>
<td>44</td>
</tr>
<tr>
<td>% due to LDRD</td>
<td>54%</td>
<td>46%</td>
<td>45%</td>
<td>47%</td>
<td>54%</td>
</tr>
</tbody>
</table>

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 Long-Term Impacts of LDRD Investments

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.
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.

<table>
<thead>
<tr>
<th>History of APS Fellows at Los Alamos National Laboratory</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Single-Year Statistics</strong></td>
</tr>
<tr>
<td><strong>FY19</strong></td>
</tr>
<tr>
<td><strong>Total awards</strong></td>
</tr>
<tr>
<td><strong>Awards with LDRD roots</strong></td>
</tr>
<tr>
<td><strong>% with LDRD roots</strong></td>
</tr>
<tr>
<td><strong>Average years from first LDRD experience</strong></td>
</tr>
</tbody>
</table>

*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
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.

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.
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

<table>
<thead>
<tr>
<th></th>
<th><strong>Single-Year Statistics</strong></th>
<th><strong>Multi-Year Statistics</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FY19</td>
<td>FY20</td>
</tr>
<tr>
<td>Total awards</td>
<td>9</td>
<td>8</td>
</tr>
<tr>
<td>Awards with LDRD roots</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>% with LDRD roots</td>
<td>56%</td>
<td>75%</td>
</tr>
<tr>
<td><strong>Average years from first LDRD investment</strong></td>
<td>6</td>
<td>5</td>
</tr>
</tbody>
</table>

*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.
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

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.
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](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 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](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

<table>
<thead>
<tr>
<th></th>
<th>FY19</th>
<th>FY20</th>
<th>FY21</th>
<th>FY11-15 (5 years)</th>
<th>FY16-20 (5 years)</th>
<th>FY11-21* (11 years)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total awards</strong></td>
<td>7</td>
<td>7</td>
<td>4</td>
<td>22</td>
<td>27</td>
<td>53</td>
</tr>
<tr>
<td><strong>Awards with LDRD roots</strong></td>
<td>6</td>
<td>7</td>
<td>3</td>
<td>19</td>
<td>25</td>
<td>47</td>
</tr>
<tr>
<td><strong>% with LDRD roots</strong></td>
<td>86%</td>
<td>100%</td>
<td>75%</td>
<td>86%</td>
<td>93%</td>
<td>89%</td>
</tr>
<tr>
<td><strong>Average years from first LDRD experience</strong></td>
<td>16.3</td>
<td>12.7</td>
<td>10.0</td>
<td>10.6</td>
<td>14.5</td>
<td>12.7</td>
</tr>
</tbody>
</table>

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

**Why does this matter?**

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)
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!

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.
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*. 
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.
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


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


Presentation Slides


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. 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., 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


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, x2e2\times80\timesa8RF, 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)


**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)


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 forefront of this emerging technology to promote beneficial applications while also informing risk assessment of misuse.

Publications

Journal Articles

Submitted to Computational and Structural Biotechnology Journal. (LA-UR-21-31781)

Conference Papers

Presentation Slides


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. 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


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

Jacob Spendelow
20200200DR

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

Publications

Journal Articles


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)


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

Carrie Manore
20210062DR

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


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)


Conference Papers


Reports


Presentation Slides


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. 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)


Posters


Other


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


Reports


Presentation Slides


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)


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

Posters

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


Conference Papers

Presentation Slides


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)


Posters

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 reimagined conventional wisdom of actinide behavior in water-mediated processes at high P-T conditions.

Publications


Xu, H. Trisulfur radical anion S3\(^{2-}\) -- A major carrier for platinum in hydrothermal fluids. Submitted to *PNAS.* (LA-UR-21-27326)


*Xu, H., X. L'xc3\(\text{x}\)c3\(\text{x}\)c3\(\text{x}\)bc, P. J. Heaney and Y. Ren. Structural behavior of a stuffed derivative of \(\text{x}\)c3\(\text{x}\)y1-\(\text{x}\)1,\(\text{x}\)2, 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**


**Presentation Slides**


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


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


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


Posters


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)


Other

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 disproportionately 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.

Journal Articles


Publications


Reports


Presentation Slides


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)


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


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)


Posters


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)


Other


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


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)


Books/Chapters

Presentation Slides


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


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)


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

Marrone, B. L. LANL Biological/Biochemical Capabilities and Technologies for\xc2¹\xa0CO2\xc2²\xa0Conversion\xc2²\xa00. (LA-UR-21-21681)


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

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

Marrone, B. L., C. R. Gonzalez Esquer and S. M. Van Cuyk. CO2 stimulated 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)


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


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

Robert Currier
20190057DR

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

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 °C. Submitted to Geochimica et Cosmochimica Acta. (LA-UR-20-29341)


**Reports**


**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)


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


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


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


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)


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

Philip Stauffer
20210948DR

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

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


**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. Computing with Spin Ice. . (LA-UR-22-20331)

**Posters**

Caravelli, F. The odd 8-vertex model via Fisher-Dubédat 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
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


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


Presentation Slides

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

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

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


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

Publications

Journal Articles


Presentation Slides


Shakya, M., E. Tran and M. B. 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

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 Picoclorum 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
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


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. B-SPICE kick-off: The big picture. . (LA-UR-21-25987)

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)


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


Posters


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


Books/Chapters

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
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)

Complex Natural and Engineered Systems
Exploratory Research
Continuing Project

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


Reports

Presentation Slides
Le, A. Y. High-Altitude Nuclear Explosion Calculation performed on Grizzly for Institutional Computing Project w20_hybplasma. . (LA-UR-21-21809)


Posters

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 fluoride 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

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
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)

Reports

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. and J. Hariharan. Exploring river and delta channel networks with RivGraph. Presented at Community Surface Dynamics Modeling System Annual Meeting,
(LA-UR-21-30437)

Posters

Other
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
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
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

Presentation Slides
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


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**


**Posters**


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
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


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

Presentation Slides
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)


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

Reports

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)


Posters


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


Reports

Presentation Slides


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)


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)


Posters

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


**Conference Papers**


Books/Chapters


Presentation Slides


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


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


Kang, Q. LBM3RT Simulation of Reactive Transport in Porous Media. . (LA-UR-21-25721)


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)

Posters


Other

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 capabilities.

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


Conference Papers

Reports

Presentation Slides
Olifer, L. and S. K. Morley. Revealing Very Fast Non-Adiabatic Radiation Belt Dynamics With the GPS Constellation. (LA-UR-21-27866)

Posters
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*


*Reports*

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


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)


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


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

Illuminating Plutonium: Spectroelectrochemistry 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 (~900°C) 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 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

Reports
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


Reports


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


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


Posters

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

Kshitij Wagh
20190441ER

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

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


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

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 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

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 (CO2). Other ramifications of this effort are evident. For example, in addition to CO2 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 (H2O) from air in arid climates, where such a resource is precious). Other potential applications include the adsorption and subsequent conversion of adsorbed CO2 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 (CO2) adsorption. A revised hypothesis that has resulted, is that externally applied E-fields can be used to enhance thermally driven CO2 reactivity and conversion chemistry. Recent reports appear to support such field-enhanced catalysis. E-field enhancement has not been applied to CO2 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*
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


Conference Papers


Reports


Presentation Slides


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

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 (CO2) 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 (CO2) 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 CO2 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 large scale is a critical challenge. 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*

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
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**


**Reports**

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


Presentation Slides

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

Posters

Goldberg, E. E. Viral Modeling. (LA-UR-20-26632)
Photochemistry of Actinides in Ionic Liquids for Advanced Separations

Janelle Droessler
20200561ECR

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

Blake Hovde  
20200562ECR

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

Publications

Journal Articles


Posters

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


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

Presentation Slides
Jonko, A. Advancing coupled fire-atmosphere research with HIGRAD/FIRETEC (w20_firetec) - 2021 Institutional Computing Annual Progress Report. (LA-UR-22-21864)
Project Description
The country’s energy and environmental security depends on effective use of the subsurface because most of our energy comes from the subsurface and most of our waste material such as nuclear, brine (produced during oil and gas extraction) and CO2, is or will be stored in the subsurface. Despite this importance, we have very little timely information on subsurface conditions that affect the performance of these systems while avoiding hazards such as induced earthquakes and leakage of waste materials. Fractures at all scales are important to the performance of subsurface systems because they form the pathways for fluid migration and because their coalescence leads to earthquakes and containment failures. We are developing a new way to measure and monitor fractures in the subsurface using background seismic noise. As seismic waves travel through fractured materials, their travel times are perturbed by how weak or strong the contacts are across the fractures. Weak fracture contacts typically indicate that permeability is increasing and decreasing material strength, while stronger contacts typically indicate decreasing permeability and increasing material strength. These relationships have been observed in laboratory samples of rocks. Observing these relationships in the Earth will substantially contribute to our effective use of the subsurface.

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


Presentation Slides

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

Molecular Multi-Actinide Cores to Model Surface Reactivity

Aaron Tondreau
20190570ECR

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

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


Presentation Slides

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


Presentation Slides


Other

Posters


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


Posters

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


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


Presentation Slides

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


Presentation Slides

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


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

*Other*

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


Identifying Geometric Constraints Imposed by Antibiotics on Biomolecular Machines

Karissa Sanbonmatsu
20210759PRD1

Project Description
The project outlined here focuses 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 (CO2) emissions by 2050. In addition, this work will help strengthen the nation's energy security by developing domestic production pathways for aviation fuel using agricultural waste products as feedstocks.
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 (CO2), 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

Presentation Slides
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 accessible 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


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


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


*Greer, S. M., *\( \backslash \text{x3c3} \text{\textbackslash y} \text{\textbackslash x} \text{\textbackslash c} \text{n} \text{\textbackslash g} \text{\textbackslash n} \text{\textbackslash o}\text{rg}, \text{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)


**Reports**


**Presentation Slides**

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


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. 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. 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. 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., S. M. Greer, B. Stein and A. J. Gaunt. LANL – UoM collaboration with S. T. Liddle. . (LA-UR-21-23256)


Posters

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


Reports

Presentation Slides
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


*Zhang, X.*, I. A. Popov, K. A. Lundell, H. Wang, C. Mu, W. Wang, H. Schn\xc3\xb1c3\xb1b6ckel, A. I. Boldyrev and K. H. Bowen. Realization of an Al\xc3\xb1e2\xc3\xb1x89\xc3\xb1xa1Al 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**


**Posters**

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


Reports

Presentation Slides


Posters

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 (CO2) 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 CO2; 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
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

Posters
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
Data Driven Accelerated Fuel Qualification for Nuclear Fuels

Tammie Nelson
20210737DI

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


Reports


Presentation Slides


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


Presentation Slides

Mechanistic Studies of Human Disease

Nicolas Hengartner
20200002CR-CNLCenters Research
Continuing Project

Project Description
This project aims at modeling biological systems using computational and mathematical methods. Biological systems are modeled at different scales: atomistic (proteins, nucleic 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


**Presentation Slides**

Fox, Z. R. Computational design and control of stochastic gene expression in single cells. . (LA-UR-21-30734)


Migliori, A. D. Slides for FNLCR collaborators. . (LA-UR-19-32620)


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-21-19792)

Sarkar, S. Spatiotemporal organization of cell signaling. . (LA-UR-20-30389)

Sarkar, S. Emergent behaviors of cellular systems. . (LA-UR-20-29880)

**Posters**


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


Reports


Sadler, J. D. Theoretical justification for heat flux limiter 0.15. Unpublished report. (LA-UR-21-24977)


**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)


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)


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. 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, Las Alamos, New Mexico, United States, 2021-04-06 - 2021-04-06. (LA-UR-21-23317)


Wang, K. Physics-informed deep learning emulator for predicting porous media flow. (LA-UR-22-22104)


Weijer, W. Viewgraph for Institutional Computing reporting: w20_hilatbg. . (LA-UR-21-21639)


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)


Other

Weijer, W. and J. Zhang. CORE inter-annual forced ocean ice simulation using E3SMv0-HiLAT-tx0.3v2 (HiLAT03). Dataset. (LA-UR-20-25544)


Posters


Jadrich, R. B. Accelerating reactive ab initio simulation via Nested Monte Carlo and Machine Learning. . (LA-UR-19-24686)

Information Science and Technology
Quantum Chemistry using Quantum Computers

Pavel Dub
20200056DR

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


Dub, P. Homochiral \xc2\xb3-CF3, -SCF3 and -OCF3 secondary alcohols: catalytic stereconvergent synthesis, bioactivity and flexible crystals. Submitted to JACS. (LA-UR-22-21454)


Reports


Presentation Slides


Cincio, L. IC report: slides. . (LA-UR-22-21699)


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. Quantum Community Detection for Reduction of the Molecular Hamiltonian in Electronic Structure Problems. Presented at ACS Spring 2021 Meeting (Virtual),
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. 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)


Prioritizing the Prior: Advanced Inversion Algorithms for Scientific Data Analysis

Brendt Wohlberg  
20200061DR

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


Conference Papers


**Reports**


**Presentation Slides**


Garcia Cardona, C. Advanced Inversion Algorithms for Scientific Data Analysis. (LA-UR-21-21830)


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)


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


Conference Papers


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)


**Reports**


**Presentation Slides**


Biswas, A. In Situ Data Reduction and Statistical Inference. (LA-UR-20-30474)


Grosskopf, M. J. In Situ Inference for Exascale Scientific Computing. Presented at Joint Statistical Meeting, Online, New Mexico, United States, 2020-08-03 - 2020-08-07. (LA-UR-20-25961)

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)


**Visualization 2020**, Salt Lake City, Utah, United States, 2020-10-25 - 2020-10-25. (LA-UR-20-27080)


Jordanova, V. K. Key Aspects of Self-Consistent Ring Current Modeling. (LA-UR-20-25791)


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)


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)


**Posters**


Symposium, Virtual, New Mexico, United States, 2021-06-07 - 2021-06-10. (LA-UR-21-24747)
Uncertainty Quantification for Robust Machine Learning

Diane Oyen
20210043DR

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.

Published


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)


Conference Papers


Reports


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)


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)


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)

The Optimization of Machine Learning: Imposing Requirements on Artificial Intelligence

Russell Bent
20210078DR

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


Conference Papers


Hijazi, H. L. and S. Gopinath. Benchmarking Large-Scale ACOPF Solutions and Optimality Bounds. Presented at Power & Energy Society (PES) General Meeting. (Denver,


Reports


Presentation Slides


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

Other

Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems

Benjamin Nebgen
20210087DR

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


Reports

*206


Presentation Slides


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)


Nebgen, B. T. My path to becoming a DOE scientist. . (LA-UR-22-21251)


Smith, J. S. Robust atomistic potentials from machine learning. . (LA-UR-21-23605)

Tretiak, S. Coherent Photoexcited Dynamics 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 Photoexcited Dynamics and Intermolecular Conical Intersections. Presented at Quantum Dynamics of Excitons and 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)


Posters


Other


Nebgen, B. T. Dataset of Molecular Orbital Energies and Densities for Organic Molecules. Dataset. (LA-UR-21-23368)


Machine Learning for Realizing Next-Generation Quantum Hardware

Michael Martin
20210116DR

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


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)


Reports


Presentation Slides

Cincio, L. IC report: slides. . (LA-UR-22-21699)

Czarnik, P. J. dvanced techniques for improving error mitigation. . (LA-UR-22-20301)


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 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)


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. 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-21-31308)

S. Cerezo de la Roca, M. V. Quantum Machine Learning Exercises. Presented at PWF School on Quantum Computing, Guatemala, Guatemala, 2021-11-29 - 2021-12-03. (LA-UR-21-31585)


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


Enabling Predictive Scale-Bridging Simulations through Active Learning

Timothy Germann
20190005DR

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
*Li, Y. W., M. Lupo Pasini, J. Yin and M. Eisenbach. A scalable algorithm for the optimization of neural network


**Conference Papers**


**Reports**


**Presentation Slides**


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)


Lubbers, N. E. Bridging Computational Scales with Machine Learning. (LA-UR-21-23836)


McKerns, M. mystic - a brief introduction. (LA-UR-19-22525)


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)


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)


Pavel, R. S., C. Junghans and T. C. Germann. Workflow Requirements for Active Learning Enabled Scale-Bridging Simulations. (LA-UR-21-20939)

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. Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures. Presented at *APS March Meeting 2020*, Denver,
Rosenberger, D. G. Using machine learning to estimate ideal/non ideal mixing in binary ionic mixtures. (LA-UR-21-21248)


Viswanathan, H. S. Reducing the Environmental Footprint of Subsurface Energy. (LA-UR-21-27612)


**Posters**


**Other**


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, Environmental 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


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**Alexandrov, B.** 


**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.** 


**Alexandrov, B.** 


**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)


**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)


Conference Papers


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. Unsupervised Phase Mapping of X-ray Diffraction


Reports


Presentation Slides

Ahmmed, B. Supervised and Unsupervised Machine Learning to Understanding Reactive-transport Data. (LA-UR-20-23812)


Alexandrov, B. Nonnegative Tensor Nets and Extraction of Latent Variables Targeting Discovery. (LA-UR-20-25418)


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)


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)


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)


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)


Posters


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


and Experiment. 2020 (12): 124007. (LA-UR-19-30102 DOI: 10.1088/1742-5468/abcaf1)


Conference Papers


ODEs. Presented at *NeuRIPS Conference*. (Vancouver, Canada, 2020-12-06 - 2020-12-12). (LA-UR-20-27785)


**Reports**


**Presentation Slides**

Aslangil, D. Denis Aslangil web-page contents (denisaslangil.com). (LA-UR-20-20826)


Kaiser, B. E., J. A. Saenz and D. Livescu. Leading-Order Analysis by Artificial Intelligence. (LA-UR-20-27102)


Livescu, D. Machine Learning for Turbulence. (LA-UR-22-20657)


Posters


Aslangil, D., D. Livescu and A. Banerjee. DYNAMICS OF TURBULENCE WITH LARGE DENSITY VARIATIONS. Presented


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 increasingly 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


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)


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)


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)


Conference Papers


Books/Chapters

Reports


Presentation Slides


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. 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. IC report: slides. . (LA-UR-22-21699)


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)


Kazi, S. S. Studying Dynamical Lie Algebras Generated by Max-Cut Hamiltonian and QAQO Mixer Hamiltonians. Presented at Student Symposium, Los Alamos, New Mexico, United States, 2021-08-04 - 2021-08-04. (LA-UR-21-27740)


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. What is Quantum Computing?. Presented at Lattice QCD, Santa Fe, New Mexico, United States, 2019-08-30 - 2019-08-30. (LA-UR-19-28787)


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)
Quantum Computing with Strontium Nuclear Qubits

Michael Martin
20200015ER

Project Description
The subcommittee on Quantum Information Science under the Committee on Science of the National Science and Technology Council published a report in September 2018 entitled “National Strategic Overview for Quantum Information Science.” Here, the economic and defense implications of developing a quantum computer are discussed. Cited applications included optimization problems, chemistry, and machine learning. Meanwhile, there is a vast gap between the capabilities of current quantum hardware and the hardware requirements of useful quantum algorithms. For example, chemistry calculations can require qubit numbers of 10,000 to 1,000,000, corresponding to error rates at the part-per-billion to part-per-thousand level, respectively (smaller error rates require fewer qubits). Therefore, an outstanding challenge is to chart a path towards these kinds of performance specifications, the realization of which may be decades in the making. Neutral atom systems, as developed here, are one promising approach. This work will explore a system comprising interacting qubits encoded in the nucleus of the alkaline earth atom strontium, which has already been extensively studied in the field of atomic clocks. The same properties that make 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


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 and sensing with ultracold neutral atoms. . (LA-UR-21-25997)


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


Topological Relation-Based Image Analysis using Graphs

Diane Oyen
20200041ER

Project Description
The analysis of technical imagery is critical to matters of national security, including tracking the sharing of technical diagrams for nuclear counterproliferation, quantifying the shapes of components in images of electronics for homeland security, and in quantifying shapes of particles in materials imaging for nuclear forensics. Computer vision, especially through the use of machine learning methods, has dramatically improved the ability to detect objects in images. However, these advances have not yet automated the understanding of information contained in hand-drawn figures, technical diagrams, and imagery produced for scientific inquiry. Our key innovation is the insight that these technical images carry little per pixel information compared with natural images (photographs and video), and that context, topology and shape provide information. By representing images as hierarchical graphs, with annotations on topological relationships, we will model the context and knowledge necessary to perform intelligent analysis of images. We will be able to find altered copies of technical diagrams, whether being shared online or in publications; match tomography images to databases of known commercial electronics; and identify common shapes in materials images for forensics.

Publications

Conference Papers


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)


Presentation Slides


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)


Scott, C. B., E. Mjolsness, D. A. Oyen, C. Kodera, M. Uyttewaal. 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

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


Conference Papers


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


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,


Smith, J. S. Robust atomistic potentials from machine learning. . (LA-UR-21-23605)


Other

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


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, 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


Presentation Slides

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


Reports


Presentation Slides
Coffrin, C. J. Reflections on Benchmarking of Quantum Accelerated Optimization. (LA-UR-21-30662)
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


Presentation Slides


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

Conference Papers


Reports


Posters
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


Presentation Slides
Pakin, S. D. Running Classical Programs on a Quantum Annealer. (LA-UR-21-23768)


Posters
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**


* **Reports**

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

Conference Papers

Reports


Presentation Slides


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

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

Reports
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

Conference Papers

Reports

Presentation Slides


*Posters*


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 (biosecurity). 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


Presentation Slides


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


Conference Papers


Books/Chapters

Reports

Presentation Slides
Bujack, R. B. Vector Field Topology. (LA-UR-21-23756)

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


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)


Conference Papers


Books/Chapters


Reports


Presentation Slides


Caravelli, F. Computing with memristive devices and networks. (LA-UR-20-29385)


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)


Posters

Other
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 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


Sharan, N., Natarajan, M. 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)


Reports


Presentation Slides


Brady, P. T. and D. Livescu. High-Order Cut-Cell Methods in Multiple Dimensions. Presented at 72nd APS DFD
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)


Posters

Statistical Learning in Cyberphysical Systems

Nathan Lemons
20190351ER

Project Description
The overarching goal of this project is to develop novel data-driven algorithms for statistical 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 and statistical learning through publications and presentations at top conferences.

Publications

Journal Articles

Keszegh, B., N. W. Lemons, R. R. Martin, D. P\text{x}c3\text{xa1}y \text{x}c3\text{xb6}g\text{y}i and B. Patk\text{xc3}\text{xb3}s. Induced non-induced poset saturation problems. Submitted to *SIAM Journal on Discrete Mathematics*. (LA-UR-20-22232)


Conference Papers


Reports


Presentation Slides
Deka, D., H. Doddi and A. Lokhov. Sample Optimal topology learning of linear dynamical systems. . (LA-UR-20-25926)


Lemons, N. W. Statistical Learning in Cyberphysical Systems. . (LA-UR-21-20316)


Posters
Impact of Mobility on Coronavirus (Covid-19) Spread

Leticia Cuellar-Hengartner
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


Presentation Slides


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 that 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


Presentation Slides


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

Posters
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)


Reports


Presentation Slides


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

Reports

Presentation Slides
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


Presentation Slides


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)

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**


**Conference Papers**

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

Volkoff, T. J. and Y. Subasi. Ancilla-free continuous-variable SWAP test. Submitted to Quantum. (LA-UR-22-21141)

Presentation Slides

Posters
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

Presentation Slides


Posters
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


Reports
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


Osthus, D. A. Fast and Accurate Influenza Forecasting in the United States with Inferno. Submitted to PLOS Computational Biology. (LA-UR-20-30384)


Presentation Slides


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)


Posters

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
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 subatomic 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 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, into 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


Conference Papers

Other
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


Reports

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)


Posters


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


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. and Y. Subasi. Ancilla-free continuous-variable SWAP test. Submitted to Quantum. (LA-UR-22-21141)

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


Reports

Presentation Slides
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. 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)

Posters
Information Science and Technology
Postdoctoral Research & Development
Continuing Project

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)

Reports

Presentation Slides
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. 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)
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
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


Conference Papers


Presentation Slides

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)


Posters


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)


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
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

Presentation Slides

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


Presentation Slides

Karra, S. Al@Sensors progress update to LDRD. . (LA-UR-21-24324)


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

Conference Papers

Presentation Slides
Computing and Engineering, Los Alamos, New Mexico, United States, 2020-10-12 - 2020-10-16. (LA-UR-20-28067)


Posters

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


Conference Papers


Books/Chapters


**Presentation Slides**


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, 2020-12-08 - 2020-12-08. (LA-UR-20-29925)

Reports


**Presentation Slides**


Posters

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


Presentation Slides

Brady, P. T., D. Livescu and N. Sharan. AI Enhanced Discretizations for High-Fidelity Physics Simulations. (LA-UR-21-29077)


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)


Wilinski, M. J. Learning of the full dynamic system state matrix from partial PMU observations. (LA-UR-22-21926)


Materials for the Future
Materials for the Future

Directed Research
Continuing Project

Proximity Effects at Meso-, Nano-, and Atomic Scales: A new Path to Quantum Functionalities

Han Htoon
20200104DR

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


Books/Chapters

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

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)


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)


Alcantara, A. R., C. A. Lane and R. M. Tutchton. Beyond GGA+U: SCAN meta-GGA on 2D Van der Waals magnet CrP\textsubscript{5}S\textsubscript{4}. Presented at UNF graduate student symposium, Jacksonville, Florida, United States, 2021-10-21 - 2021-10-21. (LA-UR-21-30325)
Control Of Microstructural Instabilities in Composites (COMIC): A Pathway to Realizing Damage Resistant Metals

Laurent Capolungo
20200182DR

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


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.


Lebensohn, R. A. Brief Overview of Polycrystal Plasticity Models. . (LA-UR-21-28799)


Schneider, M. M. Recent Advancements in Tools and Techniques for Materials Characterization in the EML. . (LA-UR-21-29078)


Quantum Photonics with Semiconductor Nanocrystals

Victor Klimov
20200213DR

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


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)


Reports


Presentation Slides

Klimov, V. I. Prospects & Challenges of Colloidal Quantum Dot Laser Diodes. . (LA-UR-21-24519)


Aging and Metastability of Delta-Phase Plutonium

Jeremy Mitchell
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. Phonons as a means for understanding Pu-Ga materials. (LA-UR-21-32114)

Rudin, S. P. How does Ga doping of \textgreek{\textdelta}-Pu affect the phonons?. (LA-UR-22-21688)

Tobash, P. H. Plutonium Materials Preparation and Processing in the New RLUB 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)

Presentation Slides


Hernandez, S. C. Understanding an Unconventional Element Known as Plutonium. (LA-UR-21-26157)
Investigating How Material’s Interfaces and Dislocations Affect Strength (iMIDAS)

Abigail Hunter
20210036DR

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


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)


Reports


Presentation Slides


Gigax, J. G. Mesopillar Compression of Cu (Set B). . (LA-UR-21-30703)


Other

Topological Quantum Materials for Robust Quantum Computing

Shizeng Lin
20210064DR

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
Lin, S. Skyrmion lattice in centrosymmetric magnets with local Dzyaloshinskii-Moriya interaction. Submitted to Scipost Physics. (LA-UR-21-32483)


**Presentation Slides**


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)


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 and sensing with ultracold neutral atoms. . (LA-UR-21-25997)


**Posters**


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


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)


Conference Papers


Posters


Richmond, S. (U) Plutonium sample processing, grain growth and extraction by hydriding. (LA-UR-19-21170)


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


*M. Soe, C. M., C. C. Stoumpos, M. Kepenekian, B. Traor \textbackslash xc3\textbackslash 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, \text{(C(NH)\textsubscript{3})(CH\textsubscript{3}NH\textsubscript{3})PB\textsubscript{x}}: 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)


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)


**Presentation Slides**


Liu, F. Heterostructures Based on 2D Materials. (LA-UR-19-31053)


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. RATIONAL DESIGN OF HALIDE PEROVSKITES FOR NEXT GENERATION GAMMA-RAY DETECTION. (LA-UR-21-24320)


Nie, W. Metal Halide Hybrid Perovskite Semiconductors for Opto-Electronic Device. (LA-UR-20-27014)


Tretiak, S. Rational design of halide perovskites for next generation Gamma-ray detection. (LA-UR-19-20464)

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)


Posters


Driven Quantum Matter: A Route Towards Novel Phases

Jianxin Zhu
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**


*Chen, A., Z. Harrell, P. Lu, E. Enriquez, L. Li, B. Zhang, P. Dowden, C. Chen, H. Wang, J. L. MacManus-Driscoll and


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 La0.95Sr0.05TiO3/SrTiO3 heterostructures. Submitted to *Advanced Materials Interfaces*. (LA-UR-21-30173)


Li, H., U. Kumar, K. Sun and S. Lin. Spontaneous fractional Chern insulators in transition metal dichalcogenides MoIr\textsubscript{3}Xa9 superlattices. Submitted to Physical Review Letters. (LA-UR-21-20020)


Books/Chapters


Reports


Presentation Slides


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)


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)


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)


Yuan, L. Tracking Charge and Energy Flow at the Nanoscale by Ultrafast Microscopy. (LA-UR-21-31385)


Zhu, J. Nonequilibrium quasiparticle dynamics in an unconventional superconductor with competing order. Presented at PIP77, Santa Fe, New Mexico, United States, 2021-11-08 - 2021-11-17. (LA-UR-21-31381)


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)


enriquez, e., H. Han, P. C. Dowden and A. Chen. Advanced Thin Film Synthesis and Functionality Design Capabilities at CINT. (LA-UR-19-24301)
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


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)


**Conference Papers**


**Books/Chapters**


**Reports**

Wang, Z. Orbital ring and Dyson sphere from recycled space debris. Unpublished report. (LA-UR-21-21291)


**Presentation Slides**


Pilania, G. Annual Report Highlight Slides for w20_MatDesign. (LA-UR-21-23502)


**Conference Papers**


**Books/Chapters**


**Reports**

Wang, Z. Orbital ring and Dyson sphere from recycled space debris. Unpublished report. (LA-UR-21-21291)


**Presentation Slides**


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. Audio/Visual. (LA-UR-20-22424)

Uberuaga, B. P. Highlights performed on LANL IC on the project w19_matprops. Audio/Visual. (LA-UR-21-24026)


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)


---

**Posters**


---

**Other**

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 Laboratory 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


Presentation Slides

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


Books/Chapters

Presentation Slides

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

Posters

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


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)


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

Nicholas Sirica
20200240ER

Project Description
Within the past decade, topological materials have gone from an exotic curiosity to the subject of the 2016 Nobel Prize in Physics. Topological semimetals (TSMs) in particular exhibit a host of striking phenomena, giving them great promise for applications including quantum computing, quantum information, and spintronics. However, despite the intense effort in this burgeoning area, it has been hard to measure clear-cut signatures of material topology. This in turn has prevented these unique materials from realizing their vast potential for novel applications. Topological chiral crystals (TCCs) are a new class of materials with substantially improved properties that make measurements of previously elusive topological phenomena possible. Optical experiments can provide clear signatures of these phenomena, putting us in an excellent position to apply our extensive expertise in optical measurements on TSMs to TCCs. Our chief innovation is thus to combine our expertise in optical studies of TSMs with the availability of newly developed topological chiral crystals to clearly reveal signatures of topology. Our studies will thus establish the unique character of these systems, providing long awaited insight and comparison to theoretical predictions that sets the stage for future studies and applications of these fascinating materials.

Publications

Journal Articles


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., 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


Other

Transition Metal Nitrides for Efficient Nitrogen Electrocatalysis

Rangachary Mukundan
20200294ER

Project Description
Nitrogen reduction reaction (NRR) to produce ammonia by the Haber-Bosch (HB) process is leaving a significant carbon footprint and accounts for ~2% of global natural gas consumption and ~3% of greenhouse gas emissions. The electrochemical production of ammonia would not only solve this problem but also provide an additional way to store the energy from intermittent renewable electricity in a feedstock/fuel. The major challenge here is finding an effective catalyst for NRR since conventional precious metal-based catalysts suffer from competing hydrogen evolution reaction and catalysts with adequate selectivity have not been discovered. In this regard, transition metal nitrides (TMNs) have many advantages over metal catalysts as ammonia formation reaction occurs between the nitrogen on the nitride and adsorbed hydrogen, removing the need for pre nitrogen adsorption on the catalyst surface. We aim to prepare a variety of transition metal nitrides and evaluate their catalytic activity towards NRR in both aqueous and non-aqueous electrolytes. We will also develop the theoretical understanding of the NRR mechanism in these TMNs and develop design principles for the synthesis of efficient NRR catalysts.

Publications

Journal Articles


Posters
Design Principles for Skyrmions in f-electron Materials

Shizeng Lin
20200357ER

Project Description
Skyrmions are particle-like objects stabilized in magnets. They are promising candidates for next-generation memory devices. It is desirable to expand the skyrmion-materials in order to optimize skyrmion properties. This research will reveal a novel mechanism for skyrmion stabilization in f-electron materials. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion materials and spintronics.

Publications

Journal Articles
Lin, S. Skyrmion lattice in centrosymmetric magnets with local Dzyaloshinsky-Moriya interaction. Submitted to Scipost Physics. (LA-UR-21-32483)


Presentation Slides
Lin, S. Topology and its electrical current control in two dimensional Moiré superlattice. Presented at Wutong Forum of The Chinese University of Hong Kong, Shenzhen, China, 2021-08-14 - 2021-08-15. (LA-UR-21-28150)

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)
Pushing Past the 100 Tesla Threshold: Designing a High Conductivity/High Strength Metallic Composite Conductor

John Carpenter
20200375ER

Project Description
Energy security is of critical interest to the Department of Energy (DOE) and is one of the three main missions for Los Alamos National Laboratory. This project will develop a new metallic nanocomposite material that will enable an increase in the upper limit of magnetic fields of 100 Tesla (T) to 120 T. Currently magnetic fields are used to characterize or look at a wide variety of energy related materials such as high temperature superconductors. For the case of high temperature superconductive materials, the underlying mechanism of electron pairing remains unknown although decades have passed since the discovery of this phenomenon. Currently, we lack magnetic fields sufficient to suppress superconductivity for the materials in which the pairing is strongest. Magnetic fields beyond 100 T would enable study of the pairing interaction that is essential for development of future high temperature superconducting materials. Understanding this phase transition would enable development of near-room-temperature superconductive materials that would reinvent our current energy grid. This reinvention would be enabled by removing the resistance in the power lines that transition power from plants to homes. This increases efficiency of distribution for all power sources from wind to nuclear to coal.

Publications

Journal Articles


Emergent Infrared Localized Surface Plasmon Resonances in Doped Spinel Metal Oxide Nanomaterials

Jennifer Hollingsworth
20200407ER

Project Description
Near-infrared light (IR) is the foundation of fiber-optics based telecommunication technologies (1300-1550 nanometer). The range of communications and information technologies impacted by IR light sources, and the resulting market for IR solid-state lighting (SSL) sources—light-emitting diodes (LEDs) and laser diodes—is expected to dramatically expand over the next 5 years. These include LEDs for proximity sensors, eye tracking and gesture recognition and lasers for optical communication, Light Detection and Ranging (LIDAR) in automotive applications and 3-Dimensional facial recognition. The ability to miniaturize light sources and to easily integrate with portable/wearable/fabric technologies is key. Nanosized plasmonic materials developed here, when coupled with nanosized quantum emitters, promise new solid-state miniaturized light sources for all of these applications, which will be critical components in a range of light-enabled, global security-relevant technologies.

Publications

Journal Articles


Presentation Slides


Posters
Measurement of Dynamic Friction via Kolsky Bar

Benjamin Morrow
20200418ER

Project Description
Friction data, especially at high rates (dynamic friction), is sparse or completely unavailable for many Laboratory-relevant materials. As a result, computational models to describe friction tend to be underdeveloped and unvalidated, decreasing confidence in simulation results. This project seeks to remedy this by 1) developing the capability to measure dynamic friction without expensive and time-consuming modifications to existing test systems, 2) validate the test technique by performing measurements at quasi-static and dynamic rates; compare with known values when possible, and generate new data where legacy testing is unavailable, and 3) mature and validate the friction models developed for a Laboratory hydrocode that is used to simulate engineering systems, improve predictive capability if necessary, and use simulations to streamline analysis of experimental tests. This program will directly contribute to filling existing gaps in experimental data, and has the potential to greatly reduce both experimental and computational uncertainties for Laboratory missions such as Stockpile Stewardship, Science Campaigns, Joint Munitions Program, and others.

Publications

Journal Articles


Conference Papers


Reports


Presentation Slides


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*


*Zhao, J., F. Qin, D. Derome, Q. Kang and J. Carmeliet.*


*Presentation Slides*


Kang, Q. Institutional computing project annual report: Figures. . (LA-UR-22-21708)


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

Presentation Slides
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

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*


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
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 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


Presentation Slides
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 (CO2)-electroreduction and electrochemical ammonia synthesis. This project focuses on controlled functionality and predictable performance through the discovery of fundamental material properties with theory-guided innovation at the boundaries of chemistry, physics, and materials science. Our team seeks to create the capability to enable process-to-performance design rooted in fundamental science through advancing our understanding of mechanisms, rates, and performance of materials.

**Publications**

*Presentation Slides*

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 tabletop 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


Presentation Slides

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. 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*


*Presentation Slides*
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*
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


Presentation Slides
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 throughout the world. Once the instrument is built and optimized, we will test the feasibility of detecting defects in commercially available batteries.

Publications

Journal Articles
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 quantities 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 actinium 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.

Journal Articles


Reports

Presentation Slides

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*


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


**Presentation Slides**


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)


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)


**Posters**


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

Posters
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


Reports
**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)


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)


**Posters**


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

Materials for the Future
Exploratory Research
Final Report

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


Presentation Slides

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*


*Presentation Slides*


*Other*

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

Reports

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...
Yoo, J. Two-dimensional Materials Research at LANL. (LA-UR-19-27080)


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


Reports


Presentation Slides

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


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

Reports

Presentation Slides
Yin, X. Advancing Electrocatalysts for Energy and Environmental Applications. (LA-UR-20-20432)


Posters
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


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


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
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

Presentation Slides
Brown, C. B. Microstructure Characterization of Additive-Manufactured PBX. (LA-UR-20-22869)

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 (TiO2)/Strontium titanate (SrTiO3); (ii) synthesize most promising TiO2/SrTiO3 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)


Reports

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
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 (Ga2O3), and diamond have the potential for far superior performance. Thus, there are strong motivations and emerging opportunities for further developing Ga2O3 semiconductors, but progress in developing Ga2O3-based semiconductor devices has been severely constrained by the availability of epitaxial Ga2O3 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 Ga2O3 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


Presentation Slides


Pandey, A. Physics-informed data-driven surrogate modeling for advancing experiments and the study of novel materials. . (LA-UR-21-27990)


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

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.
Materials for the Future
Early Career Research
Continuing Project

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
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
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


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*


*Reports*


*Presentation Slides*


*Posters*


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


Presentation Slides


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. 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. 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)
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\textregistered superlattices. Submitted to PRB. (LA-UR-21-20508)

Presentation Slides


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


Presentation Slides
Lindquist, B. A. Using Statistical Inference to Discover Interactions for Colloidal Self-Assembly. Presented at


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


Posters


Materials for the Future
Postdoctoral Research & Development
Continuing Project

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*


*Presentation Slides*


*Posters*

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*


*Presentation Slides*


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


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)

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 Moiré 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


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


Presentation Slides


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
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*

*Presentation Slides*
Materials for the Future
Postdoctoral Research & Development
Continuing Project

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


Presentation Slides
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


Presentation Slides


Reports
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
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
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., 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 Jubilee meeting, Bangalore, India, 2020-12-18 - 2020-12-18. (LA-UR-20-30343)


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


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


Presentation Slides


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
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


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)


Presentation Slides


Matzelle, M., C. A. Lane, R. He, R. S. Markiewicz and A. Bansil. An ab initio Study of Oxygen Vacancies in Ba2CuO3+\r\n\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)


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 project 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*


*Presentation Slides*


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

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

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

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)


Osborn, H. and A. Stergiou. Heavy Handed Quest for Fixed Points in Multiple Coupling Scalar Theories in the $\chi e\chi_5$ Expansion. Submitted to Journal of High Energy Physics. (LA-UR-20-27569)


Presentation Slides
Stergiou, A. Uncovering the Structure of the $\chi e\chi_5$ 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. Strongly-coupled Physics Through a Conformal Field Theory Lens (IC project w20_strongcftlens). . (LA-UR-21-21777)
Materials for the Future
Postdoctoral Research & Development
Final Report

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


Presentation Slides


Posters

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


Reports


Presentation Slides


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)


Posters


Other

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


Posters
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


Posters

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


Reports

Presentation Slides
Craven, G. T. Data-Driven Determination of Correlation Functions. (LA-UR-20-24825)


Other
Craven, G. T. Dataset and programs to calculate properties of a Lennard-Jones fluid. Dataset. (LA-UR-20-24204)
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


Presentation Slides
Materials for the Future
Postdoctoral Research & Development
Final Report

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
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


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)

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


Presentation Slides

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)
Materials for the Future
Mission Foundations Research
Continuing Project

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

Presentation Slides
Dervishi-Whetham, E. High -Performance/-Precision/-Z(HPPZ) Scintillator Grids via Advanced Electrochemistry Phase
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.
Materials for the Future
Mission Foundations Research
Final Report

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
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
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

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 semiconductor. 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


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
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
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)

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 embrittleness of the material causing reduced ductility, decreased toughness, and fracture. Hydride formation in uranium (U) metal is particularly undesirable because it causes a 70% volume expansion of the metal lattice and the hydride corrosion product uranium hydride (UH₃) is a friable, pyrophoric powder. We propose to use Ultracold Neutrons (UCNs) to probe surface hydrogen (H) distribution and accumulation, helping us to discern whether UH₃ preferentially forms at the oxide/metal interface or in U metal, away from the interface. If these experiments are successful, the apparatus will also provide an important tool to study the effect of manufacturing process (e.g. various solidification technologies vs. wrought processing) on hydride corrosion susceptibility. A successful demonstration of this technique will be of interest to the National Nuclear Security Administration. The technique can also be expanded to other Uranium-based molecules, which will provide valuable data on surface hydride formation for nuclear fuel materials.

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)
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

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


Reports

Presentation Slides


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)


Choi, Y. J. Applying Neural Networks to Experimental Diffraction Data. (LA-UR-20-26201)


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)


Sweeney, C. M. Data Science for Real-time Experimental Workflows at User Light Sources. . (LA-UR-21-24356)


Posters


Other

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


Reports


Presentation Slides

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)


Powell, M. S. Insight into the chemistry of PETN and TNT during shock compression through ultrafast absorption spectroscopies. (LA-UR-21-25141)


**Posters**


Investigation of the Role of Actinides on the Local Structure of Molten Salts Using Neutron Pair-distribution Function Analysis

Sven Vogel
20200747DI

Project Description
Molten salts play important roles in nuclear processes from actinides processing (including spent fuel processing) to cooling or fuel media for novel reactor concepts (including small modular reactors). Properties of the melts are of paramount importance to understand, control, and optimize these processes and design for these applications. Due to the temperatures involved as well as chemical and radiological hazards involved, typical characterization techniques often cannot be applied. A information gap therefore exists to characterize these materials and in particular the influence of adding actinides, such as uranium (U) and plutonium (Pu), on the properties of the melts. While modeling can close some of these gaps, experimental data to benchmark these models is scarce. This proposal closes this gap by providing data on the pair-distribution function of the melts as a function of temperature and composition, including U and Pu. Assembling a team of experts in neutron characterization and molten salts and building on Los Alamos’s unique capability to handle actinide-bearing samples, not available at other user facilities, we propose to use neutron pair-distribution function (PDF) analysis to characterize the local structure of molten salts in situ.

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


Presentation Slides

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
20210693DI

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

Enhancing Resonant Ultrasound Spectroscopy (RUS) to Measure the Elastic Properties of Complex Multi-Material Actinide Systems for In-Situ Applications

Timothy Ulrich
20210792DI

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
Method for Extending the Plutonium-238 Supply

Kirk Weisbrod
20210793DI

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.
Project Description
Characterization of the diverse process solutions at Los Alamos 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

Influence of Defects on the alpha to beta Phase Transformation in Plutonium

Sarah Hernandez
20210795DI

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

Presentation Slides
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.
**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**


Presentation Slides


Murillo, J. MS 0765 Plutonium amide molecular structure.. (LA-UR-21-29086)


Schoenemann, R. U. Thermal and magnetoelastic properties of \(\chi^{\text{fe}}\)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)


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)


Other


Schlimgen, A. W. Dataset of ab initio calculations on lanthanide and actinide molecules. Dataset. (LA-UR-21-21925)
**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**


to Nature Partner Journal Quantum Information. (LA-UR-20-22660)


Su, Y. and S. Lin. Topological Sliding Moire \( \chi \text{x\text{x}} \)1 Heterostructure. Submitted to Physical Review Letters. (LA-UR-19-30658)


Conference Papers


Books/Chapters


Gifford, B. J. Functionalized Carbon Nanotube Excited States and Optical Properties. (LA-UR-19-23110)

Reports


Presentation Slides


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 *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)


Yan, B. Information Scrambling in Complex Quantum Systems. (LA-UR-21-24337)

**Posters**


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


Conference Papers


**Reports**


Lin, S. Report for the project “Control valley polarization in two dimensional materials by electric current”. Unpublished report. (LA-UR-20-27807)


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...


**Presentation Slides**

Blaschke, D. Towards predicting material strength under extreme conditions. (LA-UR-20-27230)


Brounstein, Z. R. Thermoplastics and Thermosets Multifunctionality, 3D printing, and Accelerated Aging. (LA-UR-20-29035)


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)


Lin, S. Control valley polarization in two dimensional materials by electric current. . (LA-UR-20-27840)


Pandey, A. Physics-informed data-driven surrogate modeling for advancing experiments and the study of novel materials. . (LA-UR-21-27990)


Reichhardt, C. J. Artificial Intelligence for Dynamic Phase Transitions in Materials.. (LA-UR-20-27900)


Sirica, N. S. Resolving the Spinon Continuum. . (LA-UR-21-29850)


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


Zhang, R., H. Lin and B. Yoon. Probing nucleon strange and charm distributions with lattice QCD. Submitted to arXiv. (LA-UR-20-23850)


Conference Papers


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 - 2021-07-27). (LA-UR-21-31575)


Reports


Park, S. Note: NPR of bilinears on N_f=2+1 QCD. Unpublished report. (LA-UR-21-222575)

Presentation Slides


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. 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. 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 RFO2 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)


Hassan, M. T. Development of a New Neutron Electric Dipole Moment Experiment at LANL. (LA-UR-21-28058)


Ito, T. UCN Future at LANSE. Presented at LANSCE Future Spring Workshop, Los Alamos, New Mexico, United States, 2021-05-10 - 2021-05-10. (LA-UR-21-24476)


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)


Posters


The 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 elements 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


Conference Papers


Reports


Presentation Slides


Guardincirri, 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)


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)


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 form 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


Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in Soft-

Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in $h$ $\langle x e 2 \langle x 86 \rangle x 92 \rangle x c e \langle x b 3 \rangle x c e \langle x b 3 \rangle$ 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 $h$ $\langle x e 2 \langle x 86 \rangle x 92 \rangle x c e \langle x b 3 \rangle x c e \langle x b 3 \rangle$ Decay. Submitted to Journal of High Energy Physics. (LA-UR-20-28704)


Saxena, A. B., R. Balakrishnan and R. Dandaloff. Exact Hop $\langle x e 2 \langle x 80 \rangle x 80 \rangle$ns in a 3D Heisenberg Ferromagnet. Submitted to Physical Review Letters. (LA-UR-22-20711)


Saxena, A. B. and A. Khare. Novel Superposed Kink and Pulse Solutions for $\langle \phi \rangle$ $\langle 4 \phi \rangle$, 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 $\langle \phi \rangle$ $\langle 4 \phi \rangle$, NLS and MKdV Equations. Submitted to Physics Letters. Section A: General, Atomic and Solid State Physics. (LA-UR-22-21628)


Conference Papers


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., A. Morreale and W. E. Sonderheim. 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
Cincio, L. Fast forwarding QFTs on quantum 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. 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. 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. 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)


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)

Reports


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. 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 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. 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. 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. 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, 2021-04-06 - 2021-04-06. (LA-UR-21-23348)

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., C. Wong and W. E. Sondheim. Presentations for the 20200022DR 1st year appraisal. . (LA-UR-20-30226)


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)


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)


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. 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 Electron-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

Evgenya Simakov
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)


Conference Papers


**Books/Chapters**

Schneider, M. E. Higher-quality Sources for Electron Accelerators. (LA-UR-21-30750)

**Reports**


**Presentation Slides**


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)


Lawrence, S. K. Cu Accelerator Part Cleaning. . (LA-UR-21-26214)


Perez, D. C-Band materials modeling efforts at LANL. . (LA-UR-20-28389)


Perez, D. IC Project w20_cband FY21 highlight. . (LA-UR-22-21649)


Schneider, M. E., B. Sims, E. J. Jevarjian, A. Altmark, B. Van der Geer and S. Baryshev. Forensic Applications for THz


**Posters**


Predictive Understanding of Device Performance Through Innovative Measurement, Modeling, and Simulation on Radiochemical Dosimeters (U)

Paul Koehler
20200108DR

Project Description
Radiochemical diagnostics (aka “radchem”) have been a crucial ingredient of nuclear weapons testing since inception, and efforts continue to this day to increase their usefulness and predictive capability. We will develop a novel, innovative technique to greatly reduce uncertainties for key radchem nuclear reaction rates, thereby enabling much more predictive understanding of nuclear weapons. Almost none of these rates have been measured and so they are very uncertain. Our main goal is to solve this problem by developing the first technique capable of determining key nuclear reaction rates with the required accuracy. Once demonstrated, this capability can be applied to many more cases of high interest to radchem as well as technical nuclear forensics and nuclear astrophysics, thus impacting additional Department of Energy (DOE)/National Nuclear Security Administration (NNSA) missions.

Publications

Journal Articles


Conferences. 260: 03006. (LA-UR-21-31697 DOI: 10.1051/epjconf/20226003006)

Conference Papers

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)


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)


Posters

Revolutionary Advances in Nuclear Data to Underpin LANL 21st Century Missions

Jesson Hutchinson
20210021DR

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


Conference Papers


Reports


Neudecker, D. Test Results for Checking Reliability of Selected ENDF/B-VIII.0 Evaluated Uncertainties. Unpublished report. (LA-UR-22-21551)


Presentation Slides

Clark, A. R. Overview of dissertation and postdoctoral research. (LA-UR-21-20860)


Clark, A. R. Impact of nuclear data validation with uncertainty quantification and diverse benchmarks on criticality safety. (LA-UR-21-22043)


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. Using Machine Learning Algorithms for Large-scale Nuclear-data Validation. Presented at \( \text{xc2|xa03rd Workshop of Spanish Users on Nuclear Data on\text{xc2|xa0}} \\text{Machine Learning in Nuclear Science and Technology Applications"}\text{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\text{xc2|xa 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. 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)


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)


**Posters**


Beyond the Standard Model through Precision Neutron Decay

Steven Clayton
20210041DR

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


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)


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)


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. 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)

Mereghetti, E. beta decays to probe physics beyond the Standard Model. . (LA-UR-22-22585)

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

Luis Chacon
20210063DR

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

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

Presentation Slides
Anderson, S. E. Hohlraum Kinetic Plasma Interpenetration and Mix. . (LA-UR-22-21597)
Adaptive Machine Learning for Closely Spaced Ultra-Short Intense Accelerator Beams

Alexander Scheinker
20210595DR

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


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

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)


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 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)

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


Presentation Slides


Scheiner, B. S. Revolver 19A Omega Results. (LA-UR-19-21123)


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)

**Posters**


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


Fryer, C. L., P. Karpov and D. Livescu. Understanding Convection in the Core-Collapse Supernova Engine. Submitted to Astronomy Reports. (LA-UR-20-29683)


Tews, I., D. Lonardoni and S. Gandolfi. Chiral Effective Field Theory’s Impact in Advancing Quantum 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)


Conference Papers


Reports


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,
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)


Lippuner, J. The origin of heavy elements. . (LA-UR-18-30723)


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. Neutrinos: The Ghosts From Space. . (LA-UR-20-26425)


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)


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)


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)


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. 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)


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. 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


Other


Even, W. P. Type Ia Supernova xRAGE Simulation Data for MPA Workshop. Dataset. (LA-UR-19-27753)


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

Presentation Slides

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)

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

Presentation Slides
Neben, D. E. Ultra Wide Bandwidth Source Utilizing the Two Stream Instability. (LA-UR-21-27587)

Posters

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

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)
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


Reports


Presentation Slides


Li, F. Laser-plasma based electron acceleration and its applications. . (LA-UR-20-24276)


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


Exploration of Neutron-Star Crust Dynamics in the Era of Gravitational-Wave Astrophysics

Irina Sagert
2020014SER

Project Description
This project will quantify 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


Conference Papers

Reports


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)


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)


**Posters**


**Other**

Nuclear and Particle Futures
Exploratory Research
Continuing Project

Novel X-ray Free-electron Lasers (XFEL) Accelerator Architecture

Petr Anisimov
20200287ER

Project Description
X-ray free-electron lasers (XFELs) are billion-dollar-class scientific instruments used for discovery science in materials, biology, and chemistry, and also for national security applications. For example, Los Alamos has identified an XFEL as a potential tool to address developing a needed future capability for ensuring the viability of the nation’s nuclear assets, the dynamic mesoscale materials science capability (DMMSC). Despite their cost, the broad impact of XFELs has led to the recent development of a half-dozen XFEL facilities worldwide, including one already operating in the United States and another coming on-line in a few years. Their high cost results from electron beam instabilities in the accelerators driving the XFELs, which presently can only be mitigated by increasing the electron beam energy. This in turn requires a longer (and more expensive) accelerator. The goal of this project is to investigate if a novel accelerator architecture generating a microbunched electron beam can suppress these instabilities to the point that significantly lower electron beam energies (and thus a much less expensive accelerator) can be used to drive XFELs. If so, this approach may lead to XFELs inexpensive enough that they can become university-laboratory sized tools.

Publications

Journal Articles


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. SASE, High-Gain FEL & 1D Theory. . (LA-UR-21-20609)


Presentation Slides
MixIT – Understanding Mix in Fusion Implosions through Ion Temperature Imaging

Verena Geppert-Kleinrath
20200324ER

Project Description
This project will produce the first-ever spatially resolved ion temperature measurement of inertial confinement fusion (ICF) implosions. The novel measurement has the potential to uncover the missing piece on the path to ignition for future fusion facilities. Leveraging our expertise as world leaders in fusion neutron imaging we will enhance cutting-edge technology to determine plasma ion temperature – adding a transformational diagnostic capability to Los Alamos National Laboratory’s toolkit for fusion research. The injection of contaminant mass into fuel regions - or mix - is believed to be a primary factor preventing ignition at the National Ignition Facility - the world’s most powerful ICF facility. Knowledge of the temperature distribution in the hot spot will be crucial for determining accurate estimates of the amount of contaminant and for providing constraints on radiation-hydrodynamics modeling of ICF experiments. A better understanding of ICF burn and hydrodynamic mix does not only advance the United States fusion program, it also ties directly into our core mission of stockpile stewardship.

Publications

Presentation Slides


Birge, N. W. and V. Geppert-Kleinrath. MixIT LDRD Lens Design. (LA-UR-20-24227)

Geppert-Kleinrath, V. The Quest for Symmetry: Nuclear Imaging of Inertial Confinement Fusion Implosions. 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)


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

Mark Zammit
20200356ER

Project Description
The tokamak disruption problem poses a serious threat to the future success of the International Thermonuclear Experimental Reactor (ITER), efficiently harnessing magnetic confinement nuclear fusion energy, and understanding energy production in civilian applications. During this project we will develop the Los Alamos atomic physics suite of codes to support the plasma modeling effort to design a tokamak disruption mitigation system. Los Alamos is the ideal venue for such research, as this problem requires a cross-disciplinary synergistic approach between atomic physicists, and plasma physicists, as well as the utilization of abundant computing resources and sophisticated atomic physics tools that are only available at Los Alamos. This project will contribute to the design and implementation of a disruption mitigation system that is required in the operations of ITER and future fusion tokamak facilities. The developments made during this project will have a direct application to inertial confinement fusion experiments.

Publications

Journal Articles


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...


**Conference Papers**


**Reports**


**Presentation Slides**


Garland, N. A. Impact of a minority relativistic electron tail interacting with a thermal plasma containing high-atomic-number impurities. (LA-UR-20-23791)


How do Pulsar Winds Shine in Tera Electron Volt (TeV)?

Fan Guo
20200367ER

Project Description
This project aims at understanding the origin of multi-Tera Electron Volt (TeV) emission from pulsar wind nebulae powered by termination shocks created by relativistic pulsar winds. This is a fundamental question in our understanding of the cosmos. This project brings together theory, numerical modeling, and multi-wavelength observations including gamma-rays. It builds capabilities in particle and gamma-ray detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Publications

Journal Articles


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)


**Presentation Slides**


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. 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. Finding a gamma ray in a haystack. . (LA-UR-21-30455)


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)


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)


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

Matthew Mumpower
20200384ER

Project Description
Fission yields are important for a variety of applications and for our basic scientific understanding of the fission process and many-body nuclear physics. For nonproliferation purposes, fission fragments represent the initial conditions that decide upon the emission of neutron and gamma emission, which constitute signatures of specific nuclear materials. For nuclear forensics, fission yields are needed to identify the fuel and determine the neutron spectra that can be used to reconstruct and infer specific designs. For stockpile stewardship, fission yields are also needed to interpret historical data. For nuclear energy and nuclear waste management purposes, fission yields are needed in a large range of applications, like decay heat, shielding, dosimetry, fuel handling and safe waste disposal. They are also critical to properly perform a fission product inventory at each stage of the nuclear fuel cycle in reactors. Other applications include safeguards for nuclear reactor monitoring and medical applications for radioisotope production. This work is directed at improving the modeling capabilities needed in such applications, by implementing state-of-the art theoretical models capable of producing fission yields to be used in a variety of applications.

Publications

Journal Articles


Conference Papers

Reports


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)


Sprouse, T. M. Propagation of nuclear model uncertainties in science applications. Presented at Workshop for Applied Nuclear Data Activities, Los Alamos (virtual via WebEx), New Mexico, United States, 2021-01-25 - 2021-02-03. (LA-UR-21-20577)

Neutrino Physics with Short- and Long-baseline Experiments

Sowjanya Gollapinni
20200539ER

Project Description
Why do we live in a matter-dominated universe? The tiny, subatomic particles called "neutrinos" may hold the answer to this most sought-after question. The Deep Underground Neutrino Experiment (DUNE) which forms the United States flagship experiment aims to explore this by sending neutrinos over 800 miles from Illinois to South Dakota. Several neutrino experiments in the recent past reported anomalous results that indicate there maybe more than three types of neutrinos ("sterile" neutrinos), which if proved to be true will have significant implications to our current understanding of neutrinos. The Short-Baseline Neutrino (SBN) program at Fermilab is exploring existing hints to address this. Both of these efforts are part of the high energy physics mission for Department of Energy (DOE) Office of Science. The proposed research spans the DUNE and SBN experiments and significantly enhances their technical and physics capabilities towards achieving the above stated goals. Novel calibration techniques using a high-power laser system and a source of low energy neutral particles ("neutrons") are proposed in order to achieve the measurement precision needed for DUNE. At SBN, a rare particle production process will be studied to address the sterile neutrino question which will be a "breakthrough" result in neutrino physics.

Publications

Journal Articles


Reports


Presentation Slides

Gollapinni, S. Unlocking the Mysteries of Neutrinos with the Deep Underground Neutrino Experiment. (LA-UR-21-22367)


Gollapinni, S., M. R. Lonegran and MicroBooNE Collaboration. Neutral Current Pi0 Rate Measurement with the...

Posters


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

Presentation Slides
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

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


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:
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**


**Presentation Slides**


**Posters**

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

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 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)

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\(\times\)c\(\times\)b\(\times\)3 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. 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 and E. A. Bennett. White Source n-gamma Coincidence Measurements of gamma-Production Cross Sections at LANSCE. . (LA-UR-21-30669)


Posters
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
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 as 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

Posters
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

Presentation Slides
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.
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


Conference Papers

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


**Presentation Slides**


**Posters**


Pinning Down the Neutrino-proton Process Importance in Heavy Element Production via Reaction Studies on Radioactive Nickel-56

Hye Young Lee
20180228ER

Project Description
The entire project effort, from radioactive sample production at the Isotope Production Facility to performing neutron-induced reactions at Los Alamos Neutron Science Center, can be only performed at Los Alamos National Laboratory in the US. The project results will extend to the study of nuclear reactions on radioactive samples, directly related to NNSA missions, including radiochemical detector analysis, device diagnostics, and other areas. Through this project we will improve our understanding of nuclear reaction mechanisms with mission relevance.

Technical Outcomes
To better understand heavy element productions in core-collapse supernovae, the team measured the radioactive nickel-56 $^{56}$Ni (n,p) reaction and demonstrated the new work flow for: producing the 6-day half life $^{56}$Ni isotope, transporting to the Hotcell for chemical separation and thin film fabrication, and directly measuring (n,p) and (n,a) reaction cross sections on $^{56}$Ni and $^{59}$Ni in the neutron energy range of 0.5 -10 Mega electron-volt. for the first time.

Publications

Journal Articles


Reports


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)


Brookhaven, New York, United States, 2020-11-30 - 2020-12-04. (LA-UR-20-29936)


Posters


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 have 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


Conference Papers


Presentation Slides

Parker, L. P. 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-20-29819)

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


Liu, Z., B. Mecaj, M. Neubert and X. Wang. Factorization at Subleading Power and Endpoint Divergences in h \(e\bar{e}\)x86\(\gamma\)92\(\gamma\)ce\(\bar{e}\)x3\(\gamma\)ce\(\bar{e}\)x3 Decay: II. Renormalization and Scale Evolution. Submitted to Journal of High Energy Physics. (LA-UR-20-28938)


Vitev, I. M. and J. Lansberg. Perspectives for quarkonium studies at high-luminosity LHC. Submitted to Elsevier journal family. (LA-UR-20-28018)


Books/Chapters


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
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


Conference Papers

Reports


Presentation Slides

Huang, C. Particle accelerators: present, future and the enabling computational modeling. . (LA-UR-19-31915)


Posters


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 a 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**


**Reports**


**Presentation Slides**


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)


Posters


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 micrbunching 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 infrared pyrometer that detects the signal, and software for looking at the data.

Publications

Journal Articles


Presentation Slides

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)


Posters
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


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)


Conference Papers


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


Presentation Slides


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. 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. 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. 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 solid-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

Reports
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

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)


Posters
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

Presentation Slides
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

Presentation Slides

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.

Reports


Maldonado, A., H. R. Trellue, M. E. Blood, M. E. Rising and J. G. Richard. MCNP\xe2\x80\xaex2\xe2\x80\xaearned Multigroup Macroscopic Cross Section Capability for Griffin and Validation with Hypatia Experiment. Unpublished report. (LA-UR-21-29177)


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\xaex2\xe2\x80\xaex80 Sensitivity 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)

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


Posters

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

Presentation Slides
Kleinjan, D. W. LANL & Max Planck IPP Kickoff Discussions. (LA-UR-20-21378)

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
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


Presentation Slides
Le, A. Y. and B. A. Wetherton. VPIC Mirror Modeling Update. (LA-UR-21-26113)


Posters

Le, A. Y. Hybrid-VPIC 3D full-device magnetic mirror simulation preformed on Grizzly. (LA-UR-22-20816)

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 a 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
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., 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
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

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)

Posters
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-\gamma 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
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 always possess multilinear 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. Slow manifold reduction as a systematic tool for revealing the geometry of phase space. Submitted to Physics of Plasmas. (LA-UR-22-20125)


**Reports**


**Presentation Slides**

Burby, J. W. Integrating guiding center motion in loop space. . (LA-UR-19-22767)


Burby, J. W. Slow manifold integrators and the errors they commit. . (LA-UR-19-28965)


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)


**Posters**

Project Description
This project addresses two of the great open scientific questions of our day, which are also two of the top research priorities of the Department of Energy Office of Science: “What is the origin of the matter-antimatter asymmetry?” and “What lies beyond the Standard Model of Particle Physics?” The first question addresses the origin of all visible matter in our universe today, which cannot be explained by the current Standard Model of Particle physics, thus connecting it to the second question. Answers to these require the development of frontier theoretical and computational tools as well as experimental techniques to probe physical phenomena lying beyond the Standard Model that could provide these answers. In addition, the theoretical tools are applicable to studying other physical systems, such as supernovae and how the propagation of neutrinos through them affects the dynamics of their explosions, while the experiments develop cutting-edge technology and capabilities in accelerator science and in trapping and measuring precisely ultracold neutrons. At the conclusion of our project, besides having such new tools and capabilities, we expect to have made a major step towards understanding how the matter in the universe could have been generated in its first few moments of existence.

Publications

Journal Articles


Fuyuto, K., 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)


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. 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 to 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, or 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


Presentation Slides

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 extensible to the Laboratory's stockpile stewardship mission.

Publications

Journal Articles
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)

Presentation Slides
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. 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)


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. Presented at ANSI Seminar, Los Alamos, New Mexico, United States, 2021-10-05 - 2021-10-05. (LA-UR-21-30094)

**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. 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. Project visit LDRD 20200687PRD2. . (LA-UR-21-25276)


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. Parameter estimation for experiments in astrophysics and hydrodynamics: techniques and infrastructures.
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 United States' LIGO mission and future space-based international LISA mission.

Publications

Journal Articles


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

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)


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)


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)


Presentation Slides


Yan, B. From Precision calculation to new physics searches at colliders. . (LA-UR-21-22158)

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


Presentation Slides

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 capability for modeling of the high-energy density environment of nuclear explosions.

Publications

Journal Articles


Presentation Slides
Upton Sanderbeck, P. R. Signatures of primordial origins around supermassive black holes. (LA-UR-22-20491)

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


Conference Papers


Presentation Slides

Parker, L. P. An FPGA-based Compton Mapping Pipeline. (LA-UR-20-30237)

Posters

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


Tews, I. What can neutron stars reveal about the equation of state of dense matter? *EPI Web of Conferences*. 235: 07002. (LA-UR-20-21735 DOI: 10.1051/epiconf/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)


**Reports**

Dietrich, T. and I. Tews. Neutronensterne befl"{x}c3\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. 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. 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)

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


Conference Papers


Presentation Slides


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)


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
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
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

Presentation Slides
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*

*Presentation Slides*
Nuclear Material Control and Accounting (NMC&A)/In-line Monitoring Capability (ILM)

Rollin Lakis
20200668DI

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


Presentation Slides


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)


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

_Holly Trellue_
20190649DI

**Project Description**
Innovative nuclear reactor designs are currently being proposed to increase efficiency and economic viability of nuclear energy production. Microreactors are one example of a portable reactor concept that can provide power in remote environments. In support of these designs, moderated materials such as yttrium hydride provide reductions in the size requirements of the system. Understanding of hydrogen dynamics, i.e. the behavior of hydrogen atoms in materials as a function of temperature and hydrogen concentration, is of paramount importance for applications that assess material behavior (e.g. corrosion) of these advanced moderators. The combination of experimental results and advanced multi-physics simulation tools from this project will further our understanding and ultimately provide predictive capabilities of hydrogen behavior in a nuclear reactor. These capabilities can be applied to other hydrogen-related problems after the end of this project. A high fidelity hydrogen mapping capability will be developed at LANSCE, and a new multi-physics framework for a range of reactor design analysis will be generated.

**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*


*Conference Papers*


Reports


Presentation Slides


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

Tsuyoshi Tajima
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

Presentation Slides
Science of Signatures
Hyperspectral X-ray 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


Presentation Slides


Croce, M. P. IAEA Sample Results and Microcalorimeter Capabilities. (LA-UR-19-30668)

Croce, M. P. LANL LTD Projects. (LA-UR-19-31710)


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


Other

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


**Conference Papers**


**Reports**


**Presentation Slides**


Benedict, K. B. Investigations of Atmospheric Chemistry: Connecting the sources of emissions to impacts... (LA-UR-21-31221)


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. (U) Hot Smoke-Dust Signatures to Predict Nuclear Fallout and Winter (20200035DR) 3rd Year Review. . (LA-UR-22-20329)


British Columbia PyroCbs Match Observations of aerosol lofting and production (and BC21 PyroCb) Modeling and Simulations - Informed Hiroshima Fallout Simulations. (LA-UR-22-20287)


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. British Columbia 2021 Fire Pyrocumulonimbus HIGRAD Simulation - Visualization. (LA-UR-21-31598)


McClanahan, T. C. Study of the Production of Isotopes in an Urban Nuclear Post- Detonation Environment. (LA-UR-20-22421)


Perez, D. M. Cloud Microphysics Considerations for Simulating Pyrocumulonimbus Clouds in HIGRAD. (LA-UR-20-27338)


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


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)


Other

Capturing the Origin and Evolution of Persistence Using Real-time, In vivo, Single Cell Transcriptomics

Murray Wolinsky
20200222DR

Project Description
Antimicrobial and anticancer therapies frequently fail due to tiny numbers of cells which persist despite treatment. Current analysis (transcriptomic) methods are blind to the existence and behavior of these crucial actors (“persisters”) unless infeasible numbers of cells are employed. Improving therapies requires developing new methods. Our effort will identify and study the persisters that determine the fate of populations using novel technology developed for that purpose. Existing methods of transcriptomics are inadequate. But a radically new approach has only recently become possible: the ability to monitor the internal state of individual cells and to do this for many cells in real time. We will mature this latent technology, drawing on critical Los Alamos innovations. Our project is organized to perform foundational studies using our transformational new approach. We will observe the temporal dynamics of gene expression in single cells in vivo. Our method is called RIVOT (Real-time In VivO Transcriptomics). We will identify each gene expression event of interest by generating bar-coded signals as it occurs. We will watch expression of multiple (~10) targeted genes simultaneously. Our effort will not only provide unprecedented insight into persistence, it will revolutionize the study of gene expression in doing so.

Publications

Journal Articles


Conference Papers

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)


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

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)


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

The Mini Astrophysical Mega Electron-volt Background Observatory (MAMBO) CubeSat Mission: Demonstrating Agile Satellite Platforms for Astrophysics and National Security

Peter Bloser
20210047DR

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

Conference Papers


Reports


Presentation Slides


Posters

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
Coombs, K. E. Microphysiological Systems and Mechanobiology. (LA-UR-21-23309)

Posters

Presentation Slides
Akhadov, L. E. Summary of Research Experience. (LA-UR-21-30606)
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

Presentation Slides
Tutt, J. R. and T. C. McClanahan. Activation Calculations using MCNP Unstructured Mesh Geometries. Presented at 2021 MCNP\textsuperscript{xc2}\textsuperscript{ae} User Symposium (Virtual), Los Alamos, New Mexico, United States, 2021-07-12 - 2021-07-16. (LA-UR-21-26603)

Posters
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 outperforms 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

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. A Moving Waveguide Sagnac Atom Interferometer. Presented at Workshop on Inertial Sensing,


Kim, H. Waveguide atom interferometer at LANL. (LA-UR-21-22793)


Kurkuoglu, D. M. Quantum simulation and quantum technologies with cold atoms. (LA-UR-20-22384)


Posters


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 vari-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


Reports


Presentation Slides

Azad, A. K. HARNESSING LIGHT-METASURFACE INTERACTIONS FOR ENABLING TECHNOLOGIES. Presented at IEEE Research and Applications of Photonics In Defense Conference,


Azad, A. K. LDRD-DR appraisal. (LA-UR-20-21824)


Cardin, A. E. Dynamic Metasurfaces for Advanced Applications. (LA-UR-21-27661)


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. Metasurfaces for Manipulating Terahertz Radiation. (LA-UR-19-25954)


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)


R. Dalvit, D. A. Nonreciprocal Metasurfaces. (LA-UR-19-20945)


de Melo Kort-Kamp, W. J. Shaping photons in nonreciprocal space-time metasurfaces. (LA-UR-21-28677)


Posters


Saxena, A. B. Nonreciprocity and Broken Symmetry. (LA-UR-19-20944)

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


Reports

Presentation Slides
Mexico, United States, 2020-06-23 - 2020-06-27. (LA-UR-20-24356)


Hovde, B. and J. K. Jurss. Presentation - Computationally detecting real off-target effects of CRISPR/Cas9 using NGS data. Presented at Sequencing, Finishing, and Analysis in the Future Meeting, Santa Fe, New Mexico, United States, 2020-12-01 - 2020-12-03. (LA-UR-20-29659)


Posters


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)


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


Presentation Slides

Posters


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


Presentation Slides


Li, H. IC Project: Heating and Acceleration of Solar Wind by Parametric Decay Instability Mediated Turbulence. . (LA-UR-21-23434)

turbulence: recent advances and open questions, college station, Texas, United States, 2021-05-20 - 2021-05-21. (LA-UR-21-24830)


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)


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


Books/Chapters

Reports

Presentation Slides
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)


*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


Presentation Slides
Kim, Y. J. Atomic Magnetometers for High-precision Magnetic Measurements. . (LA-UR-21-23743)


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
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


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)

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


Presentation Slides
Miner, J. C. Combined experimental / computational characterization of small biotoxin structures. (LA-UR-21-22118)
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


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

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

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)


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
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

Posters
Project Description
Proton radiography (pRAD) typically operates in a very high density regime, acquiring 21 imaging frames on a 200-nanoseconds (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


Presentation Slides
Freeman, M. S. Charged Particle Radiography as an HED Diagnostic. Presented at 41st International 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*


*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*

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

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

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


Presentation Slides
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 (UF6) gas. NMR provides a unique multi-peak signature from enriched UF6 (uranium-235), as it is the only long half-life Uranium-isotope with a non-zero spin property. However, conventional NMR is not fieldable and cannot detect usable signals through pipes or containers. The zero to ultra-low field (ZULF) regime, 0–500 Nanoteslas (nT), has the potential for a portable/fieldable NMR technique to measure uranium enrichment. The method is non-invasive, can measure inside non-magnetic metallic packaging, and does not rely on ionizing radiation. An improved non-destructive enrichment verification technology would benefit onsite inspections of nuclear facilities worldwide.
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)

Posters
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.

Journal Articles


Conference Papers

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)


Reports

682

**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)


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. 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., 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)


**Posters**


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


Presentation Slides


Posters


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 Paleoeceanography and Potential Origins of Life on Mars. . (LA-UR-21-23229)


Posters

Other
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
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

Presentation Slides
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

Posters
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


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)


Posters
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)

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


Reports

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 and sensing with ultracold neutral atoms. (LA-UR-21-25997)


de Melo, L. F. Past and Present Research in Atomic Physics. (LA-UR-20-28126)

Discovering the 3D Structure and Dynamics of the Sun-Interstellar Medium System on a Global Scale

Daniel Reisenfeld
20190498ER

Project Description
The primary goal of this project is to understand the structure and dynamics of the Sun’s space environment (the heliosphere) and its ability to screen the Earth from damaging radiation that is ubiquitous in the interstellar medium. Notably, this radiation, particularly cosmic rays, has a strong solar cycle variation; it also represents the greatest risk to interplanetary travel by humans as well as one of the largest backgrounds in National Nuclear Security Administration-sponsored, Los Alamos-built space instruments that detect nuclear explosions around the globe. The project exploits data from the Los Alamos-led energetic neutral atom (ENA) imager on the National Aeronautics Space Administration Interstellar Boundary Explorer (IBEX) mission to “sound” the three-dimensional extent of the heliosphere by monitoring over time the response of the outer heliosphere (via ENA emission) to bursts of plasma originally ejected from the Sun. By imaging the outer heliospheric response over time, we can understand the plasma flows and thus the underlying physical processes that govern heliospheric dynamics over the solar cycle. This research builds leadership capabilities in space weather and informs the optimization of the ENA imager that Los Alamos will lead for NASA’s upcoming IMAP mission.

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


Reports

Presentations


Posters


2019 Fall Meeting of the American Geophysical Union,
San Francisco, California, United States, 2019-12-09 -
2019-12-09. (LA-UR-19-32234)
Rare Earth Fission Product Element Separations by High Speed Counter-Current Chromatography

Iain May
20200116ER

Project Description
The rare earths are a series of elements that have very similar chemical properties, rendering their separation and purification extremely challenging. The analysis of radioactive rare earth elements adds significantly to this challenge. Our goal is 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 seismoacoustic 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

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
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 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 feature for the active cloak. The team designed the basic building block through full-wave numerical simulations.

Publications

Journal Articles

Presentation Slides
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 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

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
Science of Signatures
Early Career Research
Continuing Project

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


Presentation Slides


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 (Virtual), 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)


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)


Other
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
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

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
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


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
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 Piezoelectric 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


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)


Conference Papers

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


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


Conference Papers


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-
Presentation Slides


Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Updates on LANL AM Data Analysis. . (LA-UR-20-25768)


Wachtor, A. J. In-Process Quality Control of Additively Manufactured Parts. . (LA-UR-19-21711)


Posters


**New Innovations in Microtesla Nuclear Magnetic Resonance Spectroscopy**

*Derrick Kaseman*

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*


*Presentation Slides*


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 together 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


Nasir, A. Genetic Promiscuity in the Human Microbiome. Submitted to *Science.* (LA-UR-20-20701)


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)


Books/Chapters

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

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)
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


Reports

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. Submitted 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)


Posters
Johnson, C. W. Identifying weak ground motions to characterize fault zone strain localization. Presented at SCEC Rupture and Fault Zone Obervartory Workshop,
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


Reports

Presentation Slides


Posters

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

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 (UxOy) single crystal thin films, we will build a small library of the XUV signatures. As a next step, the same laser which we use to produce the XUV light will be used to create a uranium plasma, so that with the XUV spectroscopy, we can both produce and measure signatures of the UxOy conglomerates and also time-resolve their growth. This is highly relevant for mission relevant for developing novel signatures for nuclear forensics and for analyzing nuclear debris. The general concept to do work that is typically done at x-ray synchrotron at a table-top source at Los Alamos, has many potential mission relevant applications in forensics of other hazardous materials or materials in extreme conditions.

Publications

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


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)


**Reports**


**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)


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 as 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


Posters

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


Presentation Slides

Posters


Other
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


Reports

Presentation Slides


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)


**Posters**


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

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

Posters
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.

Journal Articles

Books/Chapters

Reports

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)

Posters
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 significant 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)
Explores the potential of safeguard signatures with energy-resolved neutron imaging (ERNI) for future molten salt reactor designs.

**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 as a feasibility test and inform future efforts of possible technology gaps that need to be addressed in order to advance ERNI technology for safeguard proposals. 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, 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*
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

739
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

Presentation Slides
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

Posters
Scalable digital biosurveillance to advance pandemic science and preparedness

*Patrick Chain*
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*


*Reports*

*Presentation Slides*

*Posters*

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


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**


**Reports**


**Presentation Slides**


Engel, M. A. Development of Next-Generation Cross-Scale Equations for Magnetosphere Models. . (LA-UR-21-29914)


Guzik, J. A. A Tour of the Center of the Hertzsprung-Russell Diagram. (LA-UR-21-30720)


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)


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)


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)


Pinilla-Orjuela, M. I. Autonomous Optimization for Pulsed Neutron Generators (PNGs). (LA-UR-21-21736)


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)


Posters


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

Lisa Danielson
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


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, C. Rowe, E. Guardincerri and C. Frohlich.


Lundeen, J. A. "Dark Matter Searches with HAWC". Submitted to *PoS - Proceedings of Science.* (LA-UR-19-30002)


Conference Papers


Vassh, N., M. R. Mumpower, T. M. Sprouse and R. Surman. Probing the properties of neutron-rich actinides with...

**Reports**


**Presentation Slides**


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\xe2\x80\xe9 and melting ice: perspectives from field work and climate modeling. (LA-UR-21-25976)


Caldwell, W. K. FLAG Hydrocode. (LA-UR-19-23662)


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. 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)


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\textsuperscript{xc}x81tude comparative de la source sismique des impacts de m\textsuperscript{e}\textsuperscript{xc}x81t\textsuperscript{e}\textsuperscript{xc}x81r\textsuperscript{e}tites a\textsuperscript{xc}x80 la surface de diffe\textsuperscript{xc}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., P. Lognonn\textsuperscript{e}x3\textsuperscript{e}x9, C. Larmat, E. Rougier, Z. Lei, T. Kawamura and F. Karakostas. Numerical Simulation of an Impact-Generated Stress-Flut 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)


Hiraki, K. DREAM results with Arase, Himawari, and GPS. . (LA-UR-20-20423)


Holmes, R. M. Space traffic management & why satellites need license plates. . (LA-UR-18-31379)


Mesick, K. E. Engagement in LunaH-Map Mini-NS Detector Calibration. . (LA-UR-18-30099)


Miller, J. M. Neutrinos: The Ghosts From Space.. (LA-UR-20-26425)


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. 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)


Posters


Froment, M. Seismic Modeling of Meteorite Impacts on the Surface of Mars... (LA-UR-20-25070)


Other


Larmat, C. Answers to the quiz of Week 3 of InSight at home for teens. Audio/Visual. (LA-UR-20-23329)


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
Enabling Design Agility in a Joint Test Assembly Flight Body (U)

John Minotti
20210962DI

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.