

FY25 LDRD Project Accomplishments

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22-DR-001: Rapid T-Cell Engineering to Counter Emerging Threats

Project Overview

There is a critical need for new approaches to effectively counter emerging pathogens, especially those which do not respond to antibodies or antibiotics. T cells represent an essential element of native immune response in many of the deadliest pathogens: controlling T cell reactivity and behavior would allow for countermeasures for currently untreatable diseases from cancer to coronaviruses, especially if using a patient's own T cells (autologous) where no host rejection will occur. However, current methods for modifying T cells, e.g., FDA-approved chimeric antigen receptor T cell (CAR) approaches, require genetic manipulation and expansion which can take weeks to generate.

Instead of genetic engineering, we sought to determine if a rapid method of membrane protein delivery could generate functional CAR-T cells in a rapid, safer, cost-effective manner. Using cell free protein synthesis, we generated CAR proteins embedded in a nanodisc, and thus effectively solubilized the protein. We demonstrated the first functional CAR proteins outside of a cellular context. We next tested uptake into immune cells and found extremely high uptake into T cells and multiple other populations of immune cells. We found some evidence of cytotoxicity in vitro conferred by the nanodisc delivered protein.

Mission Impact

Our approach to T cell engineering offers a quantum leap in personalized medicine: rapid cellular engineering (1 day vs. 3 weeks) at a sustainable cost (50k vs. 500k), deployable anywhere by medical professionals (vs. requiring a manufacturing facility and expert cell technicians). The ability to engineer T cells for infectious disease therapeutics would enable treatments or even cures for the most dangerous pathogens currently facing humanity, including pathogens which have not yet emerged. Pathogens on the WHO global priority pathogen list and select agent lists are pathogens where antibiotics, protease inhibitors, vaccines and antibodies have not been proven effective: *an effective T cell response is the key determinant of survival in many of these diseases.*

T cell-based countermeasures could secure humanity against antibiotic resistant microbes, cancer, and any number of other cellular-level illnesses, and would greatly enhance national readiness for biological threats, protecting the public health and directly strengthening both our national security and bioresilience. We demonstrate a broadly applicable pipeline (analogous to the rapid development pipeline for monoclonal antibodies), where T cell receptor complements from recovered patients can be screened for ability to control pathogens, rapidly tested in isolation and in cell cultures, then immediately used to treat affected patients, enabling cures for innumerable diseases, ranging from lethal cancers to currently incurable pathogens.

Posters

Bude, Gregory, Joshua Claxton, Matthew Coleman, Claire Robertson, Wei He, and Shakiba Nikfarjam. "Cell-free expression and refolding of membrane proteins in synthetic nanodiscs." Poster Presentation at UCD Cancer Center 18th Annual Spotlight on Early Career Investigators, UC Davis, April 2024. LLNL-POST-863630.

Claxton, Joshua, Gregory Bude, Jillian McCool, Byron Vannest, William Murphy, Matthew Coleman, Claire Robertson, and Wei He. "Generation of a CAR T receptor supported in a NanoLipoProtein complex for immunotherapy." Poster Presentation at UCD Cancer Center 18th Annual Spotlight on Early Career Investigators, UC Davis, April 2024. LLNL-POST-863803.

Claxton, Joshua, Gregory Bude, Jillian McCool, Byron Vannest, William Murphy, Matthew Coleman, Claire Robertson, and Wei He. "Generation of a CAR T receptor supported in a NanoLipoProtein complex for immunotherapy." Poster Presentation at 18th Annual Spotlight on Early Career Investigators, UC Davis, April 2024. LLNL-POST-863803.

McCool, Jillian, Joshua Claxton, Timothy Vu, Gregory Bude, Byron Vannest, Wei He, William Murphy, Matthew Coleman, and Claire Robertson. "Synthesis of Chimeric Antigen Receptor NanoLipoProteins for T cell Delivery and Immunotherapy." Poster Presentation at Peptalk 2025, San Diego. LLNL-POST-871655.

Abstracts

McCool, Jillian, Joshua Claxton, Gregory Bude, Timothy Vu, Wei He, Matthew Coleman, and Claire Robertson. 2024. "Engineering Chimeric Antigen T Cells using Protein Delivery mediated by Nanolipoprotein Particles." Abstract. UCD Cancer Center Annual Retreat, LLNL-ABS-868900.

Claxton, Joshua, Gregory Bude, Jillian McCool, Byron Vannest, William Murphy, Matthew Coleman, Claire Robertson, and Wei He. 2024. "Generation of a CAR T receptor supported in a NanoLipoProtein complex for immunotherapy." Abstract. *18th Annual Spotlight on Early Career Investigators*, LLNL-ABS-863802.

McCool, Jillian, Joshua Claxton, Gregory Bude, Timothy Vu, Wei He, Matthew Coleman, and William Murphy. 2025. "Effective Chimeric Antigen T Cells Engineered with NanoLipoProtein Protein Delivery." Abstract. *Cell and Molecular Bioengineering*, (January). LLNL-ABS- 869286.

Presentations

Jillian McCool. "Racing for a Cure: Engineering CAR-T Cells for Improved Cancer Targeting." Presented at Research SLAM, LLNL, September 2024.

Patents

Robertson, Claire, Wei He, Matthew Coleman, and William Murphy. 2024. "Immuno-nanoparticles, and related cells, compositions, methods and systems." Submitted.

Records of Invention

Robertson, Claire, Matthew Coleman, and Wei He. 2023. "Protein mediated immune cell engineering." IL-13908.

22-DR-003: High-Efficiency Biomimetic Three-Dimensional Membranes

Project Overview

Today's 2D membrane architectures limit the membrane surface area packing density, resulting in low permeation rates and large device sizes. Nature addresses this challenge by utilizing 3D membrane architectures with two independent, interpenetrating flow channel systems separated by a thin functional membrane wall. Inspired by nature's membrane design, we have developed biocompatible 3D-printed, high-efficiency membranes with the goal to enable ultra-compact wearable/implantable Renal Assist Devices (artificial kidneys). To achieve this, the membrane system requires a membrane packing density significantly higher than that of conventional hollow fiber membranes (~2,000 square meter per cubic meter) with a narrow pore size distribution around 4.0–4.5 nanometer, mimicking the glomerular pore size in kidneys and ensuring 100% retention of albumin, the smallest protein (~6 nanometer) in blood. Additionally, the membrane materials must have excellent anti-biofouling characteristics.

Building on nature's strategy of using zwitterionic surface groups like phosphatidylcholine to provide a barrier for protein and cell attachment by forming a tightly bound hydration layer, we developed a bifunctional zwitterionic acrylic monomer. This monomer enables the 3D printing of nanoporous membrane structures by taking advantage of a self-organization process called polymerization induced phase separation. Phase-field simulations were performed to guide the development of the photoresist formulation and print conditions with respect to pore size and morphology. Using projection micro stereolithography and our biofouling resilient photoresist, we fabricated 3D printed gyroid membranes with membrane surface area packing densities more than 5000 square meter per cubic meter. Membrane characterization confirmed successful control over membrane pore size down to 3 nanometer with 100% rejection for ≥ 5 nanometer gold particles. Protein (fibrinogen) adsorption tests and cell adhesion experiments using porcine whole blood demonstrated the excellent anti-fouling properties of the zwitterionic acrylate resin. Flow performance tests with one-cubic-centimeter 3D membranes showed stable blood flow rates up to 20 milliliter per minute at 5 pounds per square inch pressure differential, on par or higher than commercial hemodialysis membranes. Creatinine, a waste product removed by dialysis, was used as a platform to test the waste removal efficiency of our 3D membranes. These tests revealed that our 3D membranes remove about 10% of the creatinine in a single pass at a contact time of only 5 seconds. The low flow resistance and the excellent waste removal performance are consistent with multiphysics microfluidic simulations that reveal that the flow channel architecture supports mixing by micro-vortex formation. We conclude that the waste removal efficiency of our 3D membranes is high enough to clean the entire blood of a typical patient (about 6 liter blood) in less than one hour (allowing for >10 passes, each removing 10% of the waste products) using a kidney sized (~400 cubic centimeter) 3D membrane unit. Our technology is thus expected to enable significantly shorter dialysis treatment times and wearable Renal Assist Devices. In conclusion, our technology has the potential to disrupt the dialysis industry which is a \$50 billion/year market and addresses the needs of 500,000+ Americans with total and permanent kidney failure that currently rely on ambulant hemodialysis.

Mission Impact

The development of 3D membranes addresses DOE's energy and environmental security missions and supports LLNL's mission in Advanced Materials and Manufacturing. The high efficiency biomimetic 3D gyroid membrane technology developed in this project enables 10x faster filtration and separation at a 10x smaller device volume, enabling ultra-compact filtration and separation systems. For example, ultra-compact 3D dialysis membranes have the potential to dramatically improve the quality of life of 500,000+ Americans with total and permanent kidney failure, and also directly address the armies' need for portable, higher efficiency dialysis devices. Other applications include element recovery (e.g. rare earth elements, lithium), carbon management, and energy storage and conversion.

Publications

L. Feng, S. Huang, T. W. Heo, J. Biener, *ACS Applied Materials & Interfaces* 2024, 16, 38442-38457.

M. Ma, A. Orhan, L. Feng, M. P. de Beer, A. L. Troksa, N. Hwee, T. W. Heo, J. Biener, J. Wan, J. Ye, *ACS Applied Engineering Materials* 2024, 2, 2245-2254.

L. Feng, S. Huang, D. Li, K. Wang, S. Kim, T. W. Heo, J. Biener, *Small Structures* (accepted)

Presentations

Feng, L., Wang, B., Heo, T., Biener, J. "Machine Learning-Assisted Understanding of Microstructure-Property Relationships and Multi-Property Co-optimization in Multi-Phase Materials." Computational Materials Science and Engineering Gordon Research Seminar (GRS) (Invited Presentation). Newry, ME, June 20-21, 2024.

Feng, L., Wang, B., Heo, T., Biener, J. "Machine Learning-Assisted Understanding of Microstructure-Property Relationships and Multi-Property Co-optimization in Multi-Phase Materials." Computational Materials Science and Engineering Gordon Research Conference (GRC) (Poster), Newry, ME, June 21-26, 2024.

Feng, L., Wang, B., Kim, K., Wan, S., Wood, B., Heo, T., Biener, J. "Impact of Microstructure on Mechanical Property and Multi-Property Optimization in Porous Materials." TMS Specialty Congress 2024. Cleveland, OH, June 16-20, 2024.

Hwee, N., Wang, K., Huang, S., Li, D., Degraff, W., Feng, L., Kim, S., Ye, J., Biener, J., "Additively manufactured 3D membranes for wearable renal assist device." 2024 MRS Spring Meeting, Seattle, WA, April 22-26, 2024.

Li D., Wang, K., Hwee, N., Degraff, W., Huang, S., Feng, L., Heo, T.W., Ye, J., Cheng, G., Kim, S., Biener, J. "3D Printed Biomimetic Ultralow-fouling Membranes for Ultracompact

Wearable/Implantable Renal Assist Devices.” ACS Spring Conference, San Diego, CA, March 23-27, 2025.

Patents

ROI 13812: International patent application filed Nov. 14, 2024; "Three-dimensional filtration composites and methods of manufacturing."

ROI 13891: Nonprovisional US patent application filed Oct. 4, 2023; "Skin-layered porous separators and related methods."

22-DR-004: Laser Amplification with Suppressed Amplified Spontaneous Emission

Project Overview

High-power nanosecond-pulsed solid-state lasers can be operated as a Q-switched power oscillator. The laser is pumped by diode arrays to drive the laser ions to their excited state to store energy in the gain medium. Then a “seed” emerges from spontaneous emission and experiences gain to grow in energy. The laser energy/pulse is increased by maximizing the number excited states in the gain medium. However, the main limitation in performance arises due to amplified spontaneous emission ASE which “de-pumps” the excited states before the pulse is generated.

We have developed a means of increasing the energy output of a laser by suppressing the ASE. We successfully demonstrated this principle-of-operation in a Nd:YAG oscillator. It was accomplished by including Cr⁴⁺ “saturable absorber” ions dispersed throughout the same YAG host as the Nd³⁺ laser ions. During the pumping cycle, the Cr⁴⁺ ions absorb the Nd-generated ASE such that it is suppressed. When the gain from the Nd³⁺ ions exceeds the loss of the saturable absorber and output coupling, the Cr⁴⁺ ions begins to saturate, and the gain medium then becomes transparent such that the energy is extracted in a nanosecond pulse.

In the past, the adverse impact of ASE has been reduced by deploying “edge cladding” at the sides of the gain medium (as is done for the Nd:glass gain medium slabs in the National Ignition Facility). In our new method, the ASE is equivalently suppressed equally throughout the entire gain medium by employing the aforementioned saturable absorber ions, yielding much higher gain than was previously possible. We have been building three laser oscillators, operating at progressively higher energy, achieving at first 0.03J/pulse in a 3-mm rod, then 0.2J/pulse in a 10-mm rod, a finally building a testbed employing a 20-mm rod that is nearly complete to generate >1J/pulse, with a ~20 nsec pulse width. By virtue of the basic physics involved, the 0.2J/pulse laser “rapid fires” to yield 4 consecutive 0.2J pulses, each separated by 80 microseconds. We developed a detailed physics model to describe the performance of these systems and have used this model to outline a pathway to much higher energy/pulse. This new mode of operation opens up laser designs which can meet demands of high energy with nanosecond pulse width and rapid-fire capability. Perhaps most importantly, these types of laser systems can be rendered extremely compact with easy alignment and few optics, thereby being suitable for fielded activities.

Mission Impact

Back in the 1970’s, it was first recognized that ASE is the critical limiting feature of high energy/pulse lasers, which is when edge cladding was first applied. Since then, this control pathway has been extensively engineered to the extent feasible and is now up against fundamental physics limitations. The concept of deploying a saturable absorber, instead of just a simple absorber of light (viz., edge cladding), opens up new possibilities in ultra-compact and robust designs. The types of lasers could be useful for industrial processing, remote sensing, and other activities for the DOE and DOD.

Lasers capable of high energy pulses in an ultra-compact footprint would be a gamechanger for future defensive systems. We have invented and demonstrated a new type of high energy/pulse laser

system that operates in a multi-shot "burst mode." Herein, amplified spontaneous emission is volumetrically suppressed throughout the gain medium enabling higher energy densities than was previously feasible, corresponding to the Core Competences of "Laser and Optical Science and Technology," as well as for "Advanced Materials and Manufacturing" since the gain medium is fabricated via the unique ceramics processing facility at LLNL. This type of laser system advances LLNL's Mission Area in Multi-Domain Deterrence across Integrated Deterrence; we have already begun working with the Joint Directed Energy Transition Office within the Department of Defense.

Publications, Presentations, and Patents

I Phillips, R Osborne, N Cherepy, A Drobshoff, Z Seeley, W Krupke, and S Payne, "Nd³⁺→Cr⁴⁺ energy transfer in co-doped Nd, Cr: Y₃Al₅O₁₂ garnet transparent ceramics", *Optical Materials: X* 21, 100292 (2024).

R Osborne, A Drobshoff, N Cherepy, R Beach, and S Payne, "Self Q-switched Nd,Cr:YAG transparent ceramics", *Laser Technology for Defense and Security XIX* 13029, 18-23 (2024).

Ross Allen Osborne, "Additively Manufactured Engineered Transparent Ceramics for Laser Gain Media", A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy at the University of Central Florida Orlando, Florida, April 2025.

Record of Invention

R Osborne, et al, "Laser with Uniformly Suppressed Amplified Spontaneous Emission", Record of Invention, IL-13963, March 27, 2024.

Presentation

R Osborne, N Cherepy, R Beach, A Drobshoff, W Rubink, I Phillips, and S Payne. "Additively manufactured self Q-switched Nd,Cr:YAG laser rods." International Conference and Expo on Advanced Ceramics and Composites (ICACC), Daytona Beach, FL, January 2025.

22-DR-007: Battling Long Coronavirus Disease 2019 in the Brain: Elucidating Mechanisms of Neural Dysfunction

Project Overview

Our project aimed to develop a first of its kind instrumented human neurovascular unit (NVU) that integrates the blood brain barrier (BBB) and a three-dimensional brain model on an engineered system that enables real-time monitoring of BBB and brain function with the goal of understand the long-term consequences of SARS-CoV-2 infection including contributions of direct and indirect infection. In this project, our team leveraged our 2D brain-on-chip experimental systems to evaluate direct and indirect infection outcomes while we developed our NVU. We noted significant alterations to neuronal function as a result of both direct and indirect infection of SARS-CoV-2. We successfully established a novel model of the NVU within this effort. Future work will focus on streamlining and adapting our system for BSL-3/BSL-4 containment studies and to evaluate the utility of the NVU for countermeasure assessment.

Mission Impact

(NVU) developed under this project is a unique capability to the laboratory and to the scientific community. Our NVU enables both basic and applied research for testing hypotheses in a complex cell model of the human brain. The LLNL NVU has broad applicability to our mission space, including threat assessment, therapeutic and medical countermeasure screening. Our NVU platform is of interest to multiple sponsors including the Department of Defense for threat assessment and countermeasure screening efforts.

Publications

Goshi N, Lam D, C. Bogguri et al. 2025. "Direct Effects of Prolonged TNF- α and IL-6 Exposure on Neural Activity in Human iPSC-Derived Neuron-Astrocyte Co-Cultures." *Frontiers in Cellular Neuroscience* (Feb 12). doi: <https://doi.org/10.3389/fncel.2025.1512591>. <http://library-rez.llnl.gov:2048/scholarly-journals/direct-effects-prolonged-tnf-alpha-il-6-exposure-on/docview/3165948049/se-2>.

Presentations

Goshi N, Triplett M, Alvarado J et al. "An instrumented Neurovascular Unit for Non-invasive Monitoring of Blood-Brain Barrier and Neural Function." Oral Presentation. Microphysiological Systems World Summit, Seattle, WA, 2024.

Goshi N, Triplett M, Alvarado J et al. "An instrumented Neurovascular Unit for Non-invasive Monitoring of Blood-Brain Barrier and Neural Function." Oral Presentation. Military Health System Research Symposium, Kissimmee, FL, 2024.

Enright H. "Human and rat neural microphysiological systems for recapitulation of infection dynamics and for medical countermeasure assessment." Oral Presentation. Defense Threat

Reduction Agency (DTRA) Comparing Animal Models to Organ Tissue Equivalents Workshop (CAMO), Lorton, VA, 2024.

Enright HA, Goshi N, Triplett M et al. "Human and rat neural microphysiological systems for recapitulation of infection dynamics and for medical countermeasure assessment." Oral Presentation. DTRA Chemical and Biology Science and Technology Conference, Fort Lauderdale, FL, 2024.

Patents

Fischer N, Massey T, Enright HA, Goshi N, Tooker AC, Triplett MG, Alvarado JA, Moya ML. "Systems And Methods For Instrumented Neurovascular Unit Device." IL-13964O1. Patent application# 18/774,634. Filing date: 7/16/24.

22-DR-009: Designing Asynchronous Circuits for Dynamic Machine Learning Adaptation

Project Overview

This project addresses the fundamental computing limitations of clock frequency and associated power overheads in current hardware designs that rely on traditional synchronous (or clock-based) logic by investigating the asynchronous (or clockless) microelectronics design paradigm. The project team applied asynchronous design to the application area of deep learning networks that can adapt themselves on-the-fly and without external intervention to changes in data and operating conditions. Asynchronous logic was used to build a convolutional neural network (CNN) accelerator for image classification that showed 4X – 5X higher energy efficiency and performance than the equivalent synchronous logic design. The research targeted asynchronous hardware acceleration for highly sparse (small) CNN models, with great storage efficiency. A dynamic task classifier selected the appropriate model for each environmental or operating condition that might occur with 93% accuracy, with average classification accuracy of the selected model of 85%.

Mission Impact

Low-power hardware is critical to security and science applications that require continued advancement in computing power. Autonomous computing and self-adaptation near-sensor benefit applications as diverse as climate research and drone-based monitoring. This work enabled advances in computing at the edge and low power AI accelerators.

Presentations

M. Vezzoli, L. Nel, K. Bhardwaj, R. Manohar and M. Gokhale, "Designing an Energy-Efficient Fully-Asynchronous Deep Learning Convolution Engine," 2024 Design, Automation & Test in Europe Conference & Exhibition (DATE), Valencia, Spain, 2024, pp. 1-2, doi: 10.23919/DATE58400.2024.10546579.

S. Krishnan Wan, Z., Bhardwaj, K., Whatmough, P., Faust, A., Neuman, S., Wei, G.Y., Brooks, D. and Reddi, V.J, "Automatic Domain-Specific SoC Design for Autonomous Unmanned Aerial Vehicles," 2022 55th IEEE/ACM International Symposium on Microarchitecture (MICRO), Chicago, IL, USA, 2022, pp. 300-317, doi: 10.1109/MICRO56248.2022.00033.

K. Bhardwaj, Z. Wan, A. Raychowdhury and R. Goldhahn, "Real-Time Fully Unsupervised Domain Adaptation for Lane Detection in Autonomous Driving," 2023 Design, Automation & Test in Europe Conference & Exhibition (DATE), Antwerp, Belgium, 2023, pp. 1-2, doi: 10.23919/DATE56975.2023.10136937.

T. Gokhale, R. Anirudh, J. J. Thiagarajan, B. Kailkhura, C. Baral and Y. Yang, "Improving Diversity with Adversarially Learned Transformations for Domain Generalization," 2023 IEEE/CVF Winter Conference on Applications of Computer Vision (WACV), Waikoloa, HI, USA, 2023, pp. 434-443, doi: 10.1109/WACV56688.2023.00051

Kelsey Lieberman, James Diffenderfer, Charles Godfrey, and Bhavya Kailkhura. 2023. Neural image compression: generalization, robustness, and spectral biases. In Proceedings of the 37th International Conference on Neural Information Processing Systems (NIPS '23). Curran Associates Inc., Red Hook, NY, USA, Article 3377, 77201–77241.

22-DR-010: Shock Ignition in Indirect Drive: A New Approach to High Fusion Gains

Project Overview

Shock ignition is a concept in inertial confinement fusion for igniting thermonuclear fuel with high energy gain in laser direct drive making prospect for evaluation at the National Ignition Facility (NIF). The original objective of this research was to determine the theoretical and experimental foundations of shock ignition on NIF in laser *indirect* drive and thus the potential for near-term implementation. We accomplished that mission but established that indirect drive shock ignition would require laser powers greater than ~ 1 PW and thus would be infeasible given NIF power capabilities. However, in the progression of this research, we uncovered a new class of generic laser pulse shapes that we entitled “delayed-drive”. A major feature is the potential for a thicker, more stable inflight shell as the capsule is compressing. Relative to regular NIF indirect drive with a conventional fast rise to constant peak power, delayed-drive introduces a temporary reduction in laser power after attaining the initial peak but, importantly, would be achievable with NIF’s power limits. This potentially offers enhancements in capsule stability and better symmetry control, but typically lower shell velocities and 1-D ignition margins. Such modified pulse shapes may thus allow us to realize higher fusion yields/gains providing, of course, that the capsule has sufficient margin to ignite.

The essence is that on NIF, we need velocity and ignition margin for ignition but, once ignited, we need fuel shell stability/integrity for fusion energy yield. Thus, with our present-day conventional drive pulse, do we have sufficient ignition margin/ignitability, but insufficient shell stability? (The present answer to the latter is arguably “yes”). If so, with a delayed drive pulse shape, we have the potential to trade some ignition margin for improved stability and thus realize higher fusion energy yields.

Mission Impact

In 2021, NIF obtained fusion ignition in the laboratory for the first time—a profound achievement. However, this target operates by conventional indirect drive and has not yet realized its full potential fusion energy gain/yield. This is likely because the capsules are susceptible to symmetry and stability issues. If achievable experimentally, this new laser pulse shape concept might have the potential to produce higher fusion yields in a robust target. This would then offer unique applications to stockpile-stewardship data needs and will be a valuable precursor to the high-gain targets required for inertial fusion energy. Thus, this work is central to the needs of LLNL’s nuclear-deterrence and energy missions and supports the laboratory’s core capability in high-energy-density science.

Presentations

Perkins, L. J., Di Nicola, J-M, Ho, D. D., Erickson, M. A., Spaeth, M. L., Manes, K. R., Strozzi, D. J., Williams, G. J., Lemos, N. R., Schneider, M. B. “Shock Ignition in Indirect Drive.” Bull. Amer. Physical Soc. 64th Annual Meeting of the APS Division of Plasma Physics. Spokane WA, Oct 17-22, 2022.

Perkins, L. J., Ho, D. D., Erickson, M. A., Spaeth, M. L., Manes, L. J., Millot, M., Lemos, N. R., Schneider, R., M. A., Spaeth, M. L., Manes, M. B, Di Nicola, J-M, Ludwig, J. "Investigation of Shock Ignition in Indirect Drive." 12th International Conference on Inertial Fusion Science and Applications. Denver CO, September 9, 2023.

Perkins, L. J., Ho, D. D., Millot, M., Zylstra, A., Lemos, N. R., Salmonson, J. D., Schneider, M. B., Blackfield, D. T., Scott, R. H. H., Spaeth, M. L., Manes, M. B, Di Nicola, J-M. "Assessment of the Feasibility of Shock Ignition in Indirect Drive." Bull. Amer. Physical Soc. 65th Annual Meeting of the APS Division of Plasma Physics. Denver, CO, November 1, 2023.

Perkins, L. J., Ho, D. D., Scott, R. H. H., Millot, M., Lemos, N. R., Salmonson, J. D., Schneider, M. B., Pollock, B., Blackfield, D. T. "Delayed-drive laser pulse shapes on the National Ignition Facility: The potential to trade ignition margin for improved stability and lower adiabat." Bull. Amer. Physical Soc. 66th Annual Meeting of the APS Division of Plasma Physics, Atlanta, GA, October 7, 2024.

22-DR-011: Ultra-High Water Recovery Desalination with Record Thermodynamic Efficiencies

Project Overview

Flowable carbon slurries enable promising electrochemical technologies for water desalination and energy storage, but their performance depends critically on maintaining both good flow properties and electrical connectivity—a challenging balance that has lacked systematic design rules. This project developed a comprehensive toolkit to understand and optimize these competing requirements. We created six complementary capabilities: (1) a rapid centrifuge-based method to measure the electrical conductivity of packed carbon slurries, enabling fast screening of different carbon mixtures; (2) systematic studies revealing that common laboratory peristaltic pumps can irreversibly damage carbon particles during circulation, fundamentally altering device performance; (3) a novel miniature jet pump that circulates slurries without mechanical contact, preserving particle integrity; (4) comprehensive mapping of how surfactants affect slurry properties, identifying critical concentrations where electrical networks catastrophically collapse; (5) direct visualization revealing that controlled gravitational settling can enhance local carbon concentrations by 30-fold at electrodes while maintaining flow; and (6) a simple fabrication method for titanium nitride (TiN) coated titanium current collectors that dramatically reduce electrical losses at interfaces.

Our results provide a unified framework for designing carbon slurry electrodes, revealing unexpected synergies (carbon black/activated carbon mixtures high in carbon black content outperform pure components by 30 percent), hidden failure modes (peristaltic pumps fragmenting particles), and counter-intuitive optimization strategies (leveraging settling rather than fighting it). The centrifuge conductivity method has also been introduced as a standard characterization tool. Together, these advances accelerate development timelines for formulation screening, eliminate common but unrecognized sources of irreproducibility, and enable rational design of flow-electrode capacitive deionization (FCDI) and electrochemical flow capacitor (EFC) systems that are critical for water treatment and grid-scale energy storage.

Mission Impact

This project directly advances Department of Energy (DOE) and National Nuclear Security Administration (NNSA) missions in energy and water security by developing transformative electrochemical technologies essential for infrastructure resilience. The rapid screening methods and particle-preserving pumping technologies accelerate development of FCDI systems for distributed, energy-efficient water treatment at DOE facilities, military installations, and critical infrastructure vulnerable to contamination or natural hazards. The TiN-coated current collectors and optimized slurry formulations enhance EFCs for grid-scale energy storage, providing rapid-response capabilities essential for grid resilience. This work exemplifies NNSA's commitment to developing science and technology capabilities that meet future national security challenges while providing immediate solutions for next-generation electrochemical systems.

Peer-Reviewed Publications

Y. M. Alkhulaifi, S. Paul, T. M. Jaroslowski, S. A. Hawks, J. G. Santiago, "A simple centrifuge cell method for *ex situ* quantification of electrical conductivity of slurry electrode materials," *Chemical Engineering Journal*, vol. 513, 162815, 2025. DOI: 10.1016/j.cej.2025.162815.

Y. M. Alkhulaifi, T. M. Jaroslowski, S. Paul, S. A. Hawks, J. G. Santiago, "A miniature jet pump for slurries," *Chemical Engineering Journal*, vol. 503, 158293, 2025. DOI: 10.1016/j.cej.2024.158293.

S. Paul, Y. M. Alkhulaifi, T. M. Jaroslowski, S. A. Hawks, J. G. Santiago, "Effects of Particle Mixing and Gravitational Settling on Charge Transport in Carbon Flow-Electrode Cells," *ACS Environmental Science & Technology*, vol. 59, pp. 3518–3526, 2025. DOI: 10.1021/acs.est.4c13987.

S. A. Hawks, "A New Method for Creating Structured High-Performance Current Collectors for Electrochemical Applications," *Advanced Engineering Materials*, 2401827, 2024. DOI: 10.1002/adem.202401827.

Conference Presentations and Posters

S. A. Hawks, J. Rivera, A. Overland, E. Krall, M. Cerón-Hernandez, S. Chandrasekaran, "Structured Current Collectors and Slurry Formulation for Flow Electrodes." Telluride Workshop on Electrochemical Separations, Telluride, CO, 2025.

S. Paul, Y. Alkhulaifi, T. Jaroslowski, S. A. Hawks, J. Santiago, "Particle Dynamics in Flow-Electrode Cells." Bulletin of the American Physical Society, 2024.

E. Krall, A. E. Overland, J. Rivera, M. R. Cero'n, S. A. Hawks, "Gas-Nitrided Titanium Current Collectors for Electrochemical Applications." Electrochemical Society Meeting Abstracts PRiME 2024, Abstract 3507, 2024.

A. E. Overland, M. R. Cerón, S. A. Hawks, "Surfactant Control of Carbon Slurry Networks, 244th Electrochemical Society Meeting. Gothenburg, Sweden, 2023.

M. R. Cero'n, A. E. Overland, S. A. Hawks, "Flow-Electrode Capacitive Deionization Performance Optimization," 244th Electrochemical Society Meeting. Gothenburg, Sweden, 2023.

22-DR-016: Converting Air into Ammonia via Advanced Manufactured Electrochemical Reactors

Project Overview

One of the most important inventions in human history is *atmospheric alchemy*: the process that allows us to turn nitrogen in air into ammonia, the key ingredient to make synthetic fertilizer. Almost half of the global population – over 3.8 billion people – live on food grown using synthetic nitrogen fertilizers. Over 90% of the ammonia produced today comes from one chemical reaction: the Haber-Bosch process, which requires high pressures and temperatures to produce ammonia and requires massive capital investment to create a new facility. As a result, the Haber-Bosch consumes around 2% of the world's energy supply and about 4% of the world's natural gas production, rendering the current way of ammonia synthesis unsustainable.

To respond to this challenge, our team at LLNL has successfully developed a novel approach to produce ammonia from nitrogen at ambient conditions. Using advanced manufacturing (AM), we have designed electrochemical reactors to successfully demonstrate the nitrogen oxidation reaction (NOR), which is the key for our development of a process to disrupt the production of commercial grade fertilizer. We used high performance computing (HPC) to perform hybrid quantum calculations and identify the key rate-limiting steps for both NOR and the nitrate reduction reaction (NO₃RR). We designed and built a state-of-the-art experimental lab that allowed us to detect and measure all of the products of these reactions, as well as develop an AM electrochemical reactor design that overcame the inherent slow diffusion of nitrogen to the catalyst surface. For NOR, we discovered that the combination of the correct metal oxide electrode and aqueous electrolyte leads to activation of the nitrogen molecule, resulting in at least one order of magnitude greater reactivity than any other results published to date. For NO₃RR, we utilized a thin film metal catalyst to successfully produce ammonia from nitrate, leading to a new project direction to remove waste nitrate from polluted groundwater and wastewater streams. Overall, in the past three years, our project not only successfully delivered on our goal of developing a new approach to produce fertilizer from air, but also established a new field of electrocatalysis, advanced reactor design for addressing real-world problems, and opened two exciting directions (fertilizer and wastewater treatment) for us to pursue with this technology.

Mission Impact

This project has explored and begun to address solutions to emerging security challenges associated with critical materials and fertilizer and food security, a key focus for Global Security and LLNL. The Air to Ammonia project established LLNL as a world leader in nitrogen electrochemistry and resulted in a premier experimental electrochemistry lab facility that now supports several other LDRD and external project teams. Furthermore, this project strengthened LLNL's reputation in AM reactor design, electrocatalysis, HPC applications, and agricultural technology, both in the state of California and across the world. Finally, this project directly addresses both Department of Energy (DOE) and Department of Defense (DOD) missions. For DOE, this project supports driving innovation in ammonia and fertilizer manufacturing in the U.S. to build a resilient domestic supply for American farmers. For the DOD, this project has gained the support of the Defense Advanced

Research Projects Agency (DARPA) through a follow-on grant award to produce ammonia as an alternative energy carrier.

Publications

Prajapati, Aditya, Alexandra Zagalskaya, Natalie Hwee, Jonathan Davis, Hui-Yun Jeong, Jennifer Moreno, Jenna Ynzunza, Sneha Akhade, and Jeremy Feaster. 2025. "Decarbonizing nitrogen fertilizer production via the electrochemical nitrogen oxidation reaction." *Chem Catalysis* 5, no. 2 (February): 101220. <https://doi.org/10.1016/j.checat.2024.101220>. LLNL-JRNL-2006014.

Prajapati, Aditya, Alexandra Zagalskaya, Natalie Hwee, Eric Krall, Jonathan Davis, Sneha Akhade, and Jeremy Feaster. 2025. "Overcoming fundamental challenges of the electrochemical nitrogen oxidation reaction." *Chemical Communications* 61, , no. 100 (November): 19796-19809. <https://doi.org/10.1039/d5cc03295d>. LLNL-JRNL-2006014.

Presentations

Jeremy Feaster, 2023, "Building Catalysts, Reactors and Engineers for a Sustainable Future." (Presented at American Institute of Chemical Engineers (AIChE) Annual Conference, Orlando, FL, November 2023).

Jeremy Feaster, 2023, "Building Catalysts, Reactors and Engineers for a Sustainable Future." (Presented at Virginia Tech Chemical Engineering Invited Seminar, Blacksburg, VA, October 2023).

Jeremy Feaster, 2024, "Building the Next Generation of Electrochemical Reactors through Advanced Manufacturing." (Presented at Penn State Chemical Engineering Invited Lecture, Livermore, CA [virtual presentation], April 2024).

Jeremy Feaster, Aditya Prajapati, Natalie Hwee, Jonathan Davis, Daniel Corral, Josh DeOtte, Victor Beck, Sarah Baker, Sneha Akhade, Eric Duoss, 2023, "Building the Next Generation of Electrochemical Reactors through Advanced Manufacturing." (Presented at American Institute of Chemical Engineers (AIChE) Annual Conference, Orlando, FL, November 2023).

Alexandra Zagalskaya, Aditya Prajapati, Natalie Hwee, Jonathan Davis, Sneha Akhade, Jeremy Feaster, 2023, "Elucidating the Mechanisms of Electrochemical Nitrogen Oxidation Reactions (NORs) on Metal Oxides." (Presented at American Institute of Chemical Engineers (AIChE) Annual Conference, Orlando, FL, November 2023).

Natalie Hwee, Aditya Prajapati, Jonathan Davis, Huiyun Jeong, Alexandra Zagalskaya, Sneha Akhade, Jeremy Feaster, 2023, "Engineering Reactors for the Electrochemical Nitrogen Oxidation Reaction via Advanced Manufacturing." (Presented at American Institute of Chemical Engineers (AIChE) Annual Conference, Orlando, FL, November 2023).

Alexandra Zagalskaya, Sneha Akhade, Jeremy Feaster, 2024, "Insights into the Electrochemical Reduction of Nitrate on Metal Surfaces." (Presented at ECS PRiME, Honolulu, HI, November 2024).

Patents

Feaster, Jeremy, Sarah Baker, Daniel Corral, and Eric Duoss. 2024. "Advanced manufactured vapor-fed electrochemical reactor (AM-VFR) for improved performance for electrochemical conversion." United States of America Patent US12146234B2, filed 9/02/2020, and issued 11/19/2024.

Feaster, Jeremy, Roger Aines, Sneha Akhade, Patrick Campbell, Maira Hernandez, Jonathan Davis, Sarah Baker, and Eric Duoss. 2024. "Direct conversion of air to ammonia via advanced manufactured electrochemical reactors." Filed.

22-ERD-049: Radiation Defect Engineering in Two-Dimensional Nanomembranes

Project Overview

Novel multifunctional membranes with controlled properties are needed for several energy-related applications, including lithium-sulfur batteries and Li extraction from seawater. However, the search for such multifunctional membranes with cost-effective and readily scalable technologies has proven to be challenging. The goal of this project was to investigate fundamental radiation defect processes in two-dimensional hexagonal boron nitride (BN) nanomembranes with properties tuned for these emerging energy-related applications. The project involved BN film deposition, material characterization, and Li electroplating experiments as well as atomistic, molecular dynamics, and mesoscale modeling. We performed the synthesis of BN films by chemical and physical vapor deposition and studied radiation damage buildup and Li diffusion in both as-grown and ion-irradiated BN films. This project developed a reactive sputter deposition process for the fabrication of non-epitaxial BN films with controlled composition, microstructure, and residual stress. We performed a series of ion bombardment experiments mapping the radiation damage buildup in both BN bulk and thin films as a function of ion dose and collision cascade density. This project contributed to a better understanding of radiation processes in group-III nitrides, with impact on a wide range of energy-related applications such as batteries, ion extraction, and desalination which would benefit from novel inorganic nanomembranes. The film deposition task of this project also evaluated the fabrication of BN as an alternative ablator for inertial confinement fusion and high-energy density physics applications.

Mission Impact

This project focused on the material development to address DOE's energy and environmental security missions and to develop science and technology tools and capabilities to meet future national security missions. It advanced our core competency in advanced materials and manufacturing, with potential technological implications for energy-related applications and inertial confinement fusion programs. This project involved the science and technology that helped position the Laboratory to support emerging needs and provided opportunities for program growth.

Publications:

Y. Zhou, S. O. Kucheyev, and L. F. Wan, First-principles elucidation of defect-mediated Li transport in hexagonal boron nitride, *Physical Chemistry Chemical Physics* (2025, accepted).

M. Seo, L. B. Bayu Aji, S. C. Kim, Y. K. Tzeng, A. A. Baker, F. M. O'Neill, S. Chu, and S. O. Kucheyev, Damage buildup in multilayer hexagonal boron nitride films under Ar ion bombardment, 2025. *Scripta Materialia* Volume 265, 1 August 2025, 116756 <https://doi.org/10.1016/j.scriptamat.2025.116756>

M. Seo, L. B. Bayu Aji, L. Zepeda-Ruiz, S. C. Kim, Y. K. Tzeng, S. Chu, and S. O. Kucheyev, Dynamics of radiation damage buildup in ultrathin hexagonal boron nitride under ion irradiation, 2025.

Presentations:

S. O. Kucheyev, "Radiation defect dynamics in semiconductors" (invited talk). The 26th International Conference on the Applications of Accelerators in Research and Industry (CAARI-2022). Denton, Texas, USA. November 3, 2022.

M. Seo, "Plasma-assisted PVD of polycrystalline h-BN films." 2024 Spring MRS Meeting, Seattle, Washington, USA. April 23, 2024.

Y. Zhou, "Multiscale modeling of phase evolution and Li-ion transport kinetics in boron nitride membranes." 2024 Spring MRS Meeting, Seattle, Washington, USA. April 25, 2024.

M. Seo, "Plasma-assisted PVD of polycrystalline h-BN films." The International Conference on Metallurgical Coatings and Thin Films (ICMCTF-2024). San Diego, California, USA. May 20, 2024.

S. O. Kucheyev, "Sputter deposition of boron-based films for energy-related applications" (invited talk). The 28th AACGE Western Section Conference on Crystal Growth & Epitaxy. Fallen Leaf Lake, California, USA. June 11, 2024.

S. O. Kucheyev, "Radiation defect engineering in hexagonal boron nitride" (invited talk). The 27th International Conference on the Applications of Accelerators in Research and Industry (CAARI-2024). Fort Worth, Texas, USA. July 23, 2024.

S. O. Kucheyev, "Dynamics of radiation defect accumulation in non-metallic materials." (invited talk). MS&T24 Technical Meeting and Exhibition. Pittsburgh, Pennsylvania, USA. October 9, 2024.

M. Seo, "Radiation defect engineering in hBN films." 2024 Fall MRS Meeting, Boston, Massachusetts, USA. December 2, 2024.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD program under Project No. 22-ERD-049.

22-ERD-050: Gas-Bubble Management for Electrochemical Systems

Project Overview

Gas evolving electrochemical reactors can boost the efficiency and productivity of industrial chemical processes. Given that many of these processes are energy and resource intensive, significant advances in this field would help assure American energy dominance. This project investigates a key limitation and shutdown mechanism for electrochemical reactors: The entrapment of and failure to remove gas bubbles from the electrode pores. By leveraging Lawrence Livermore National Laboratory's (LLNL) core competencies in advanced manufacturing and high performance computing, this project built state of the art tools to directly study the formation and transport of gas bubbles in electrochemical systems. These processes were simulated using a combination of atomistic and continuum scale models, and validated with direct observation of gas bubbles in custom 3D printed cells. From these capabilities, this LDRD was able to describe how the microarchitecture of the electrode can be tuned to modify the departure and removal of gas bubbles and establishes a framework for rationally designing gas evolving electrodes.

Mission Impact

The modeling and characterization tools developed from this LDRD enhance the fundamental understanding of gas bubble formation and removal. These tools inform reactor design strategies, which are critical to improving the performance of electrochemical devices. The knowledge gained from this LDRD is therefore directly applicable to the DOE's energy and environmental security missions. Furthermore, the capabilities developed in this LDRD are generalizable, and can be applied to any system impacted by the presence of gas bubbles, such as electroplating. Thus, the science and technology tools and capabilities developed in this LDRD can be applied to meet future national security challenges involving surface science and manufacturing.

Publications, Presentations, and Patents

Aydin, Fikret, Hawi Bacha Gameda, Henry Yu, Tiras Y. Lin, Jonathan T. Davis, and Shinyoung Kang. "Bridging the Gap: Unraveling the Mechanisms of Nanobubble Detachment from Electrode Surfaces." *ECS Meeting Abstracts* MA2024-01, no. 47 (2024/08/09 2024): 2613. <https://doi.org/10.1149/MA2024-01472613mtgabs>. <https://dx.doi.org/10.1149/MA2024-01472613mtgabs>.

Davis, J. T., B. S. Jayathilake, S. Chandrasekaran, J. J. Wong, J. R. Deotte, S. E. Baker, V. A. Beck, *et al.* "3d Printed Optimized Electrodes for Electrochemical Flow Reactors." *Sci Rep* 14, no. 1 (Sep 30 2024): 22662. <https://doi.org/10.1038/s41598-024-71765-w>. <https://www.ncbi.nlm.nih.gov/pubmed/39349533>.

Davis, Jonathan T., Kansas Seung, Jack Guo, Thomas J. Ferron, Fikret Aydin, Joshua Aaron Hammons, Tiras Y. Lin, and Shinyoung Kang. "Modeling Gas Bubbles in Water Electrolyzers across Length Scales." *ECS Meeting Abstracts* MA2024-02, no. 45 (2024/11/22 2024): 3187. <https://doi.org/10.1149/MA2024-02453187mtgabs>. <https://dx.doi.org/10.1149/MA2024-02453187mtgabs>.

Davis, Jonathan T., Kansas Seung, Joshua Aaron Hammons, Thomas J. Ferron, Swetha Chandrasekaran, Sarah Baker, Eric B. Duoss, Shinyoung Kang, and Tiras Y. Lin. "Enhanced Transport in Electrochemical Reactors Using Advanced 3d Printed Electrodes." *ECS Meeting Abstracts* MA2023-02, no. 42 (2023/12/22 2023): 2108. <https://doi.org/10.1149/MA2023-02422108mtgabs>. <https://dx.doi.org/10.1149/MA2023-02422108mtgabs>.

Guo, Jack, Tiras Y. Lin, Kansas Seung, and Jonathan T. Davis. "Bubble Transport in Porous Media for Electrochemical Applications." *ECS Meeting Abstracts* MA2024-01, no. 45 (2024/08/09 2024): 2511. <https://doi.org/10.1149/MA2024-01452511mtgabs>. <https://dx.doi.org/10.1149/MA2024-01452511mtgabs>.

"Bubble Transport with Applied Flow through a Porous Lattice for Electrochemical Applications." Postdoc Summer Slam (2024/08 2024).

Hammons, J. A., S. Kang, T. J. Ferron, F. Aydin, T. Y. Lin, K. Seung, P. Chow, Y. Xiao, and J. T. Davis. "Nanobubble Formation and Coverage During High Current Density Alkaline Water Electrolysis." *Nano Lett* 24, no. 43 (Oct 30 2024): 13695-701. <https://doi.org/10.1021/acs.nanolett.4c03657>. <https://www.ncbi.nlm.nih.gov/pubmed/39412343>.

Kang, S., F. Aydin, H. Yu, J. Guo, Tiras Y. Lin, J. A. Hammons, T. J. Ferron, K. Seung, and Jonathan T. Davis. "Modeling Gas Bubble Cycles from Nucleation to Transport in Electrochemical Systems." E-MRS 2024 Fall Meeting, 2024/09 2024).

22-ERD-051: Engineering a Biosynthetic Pathway for Glycolonitrile, a High-Energy-Material Precursor

Project Overview

Glycolonitrile (GN) is an important precursor in the synthesis of energetic materials that are critical to U.S. national security interests; however, a robust domestic supply of GN is currently lacking. To contribute toward domestic, supply chain resilience for GN, we developed a biosynthetic pathway—comprising an engineered cytochrome P450 enzyme called CYP79, its partner reductase, and an engineered aldoxime dehydratase, Oxd, enzyme—that produces an *o*-benzyl protected GN from a *o*-benzyl protected serine, a bio-renewable substrate. Our results demonstrate the feasibility of GN biomanufacturing in a non-toxic, cyanide-free process, which has the potential to encourage domestic GN manufacturing.

Mission Impact

This project is well-aligned with LLNL's BioResilience Mission Focus Area, specifically addressing the biomanufacturing of critical materials for national security needs and supply chain resilience. This project has developed new capabilities in protein engineering, including a cutting-edge design-build-test-learn protein engineering pipeline that integrates experimentation and computation. For DOE/NNSA and DOD, this work directly addresses supply chain concerns for relevant energetic materials and advances U.S. strategic competitiveness in biotechnology and biomanufacturing.

Presentations:

Moreno, M. V.; Wackelin, D. J.; Lau, E. Y.; Ortiz, E. G.; Malfatti, S. A.; Vergez, L. M.; Park, D. M.; Overton, K. W.; Zuckerman, N. B.; and Yung, M.C. "Engineering a biosynthetic pathway for glycolonitrile, a high-value chemical feedstock." 2024 Society for Industrial Microbiology and Biotechnology (SIMB) Annual Meeting, Boston, MA, 5 August 2024. LLNL-POST-867518

Wackelin, D. J.; Moreno, M. V.; Ortiz, E. G.; Malfatti, S. A.; Vergez, L. M.; Lau, E. Y.; Zuckerman, N. B.; and Yung, M.C. "Safe, efficient, domestic synthesis of glycolonitrile enabled by biocatalysis." DOD Energy and Environment Innovation Symposium 2024, Washington, DC, 4 December 2024.

Yung, M. C. "Engineering a biosynthetic pathway for glycolonitrile, a high energy material precursor." DOD/DOE Joint Munitions Program Fall 2024 Meeting, Livermore, CA, 18 September 2024. LLNL-PRES-869112

Patents:

Yung, M. C.; Zuckerman, N. B.; Moreno, M. V.; Wackelin, D. J.; Lau, E. Y.; and Ortiz, E. G. 2024. "A chemoenzymatic method to produce glycolonitrile." LLNL Record of Invention, IL-13993.

22-ERD-052: High Accuracy at Low Cost: Using Machine Learning to Emulate the Department of Energy's Global Cloud-Resolving Climate Model

Project Overview

Earth System Model predictions suffer from uncertainty due to their inability to resolve storms and topography. The LLNL-led Simplified Cloud-Resolving E3SM Atmosphere Model (SCREAM) solves this resolution problem but is too expensive to run for more than a few years at a time – which is not long enough to accurately identify patterns within chaotic weather. By partnering with the Allen Institute for Artificial Intelligence (Ai2), this project has developed an emulator for SCREAM and for the older E3SM atmosphere model. An emulator is an AI-based twin of the physics-based model which is much faster and more computationally efficient. The original plan for this project was to add a new AI-based process to a low-resolution version of SCREAM which continuously nudges it to the high-resolution answer. We implemented this approach and wrote a paper about its impact, but – as is typical for AI – the state of the science has shifted since we wrote our proposal and we ended up pivoting to directly emulating E3SM atmosphere output using a Spherical Fourier Neural Operator (SFNO) approach. In the last few months of the project, we expanded this second approach to include an interactive AI-based ocean model. This project was very successful and ultimately led to a direct LLNL funding increase to continue this work as part of the E3SM project. The SFNO model created by this project has become E3SM's official emulator and was recently featured as a highlight by BER to the DOE Office of Science. Our original nudging-based emulator is serving as the template for future incorporation of AI codes into the E3SM model.

Mission Impact

This project supported LLNL's Earth-Energy System Resilience MFA - and U.S. severe weather planning more generally - by improving the accuracy of the Earth System model predictions that underpin all such research. It drew upon and grows the Lab's core competencies in Earth and Atmospheric Science and High Performance Computing, Simulation, and Data Science. Knowledge transfer from Ai2 was essential for keeping LLNL at the cutting edge of AI for Earth System Modeling. In particular, based on this work PI Caldwell was asked to join advisory panels for Ai2 and NVIDIA's Earth System AI program as well as serving as one of four co-chairs on BER's Earth System Modeling AI planning team.

Publications, Presentations, and Patents

Peter Caldwell. "Earth System Prediction at LLNL." Presentation, to Geraldine Richmond, Under Secretary for Science and Innovation at the Department of Energy, Livermore, CA, June 23, 2023.

Peter Caldwell. "The E3SM Atmosphere Model in C++ (EAMxx)." Presentation, Energy Exascale Earth System Model Workshop, Denver, CO, June 20, 2023.

Duncan, J. P. C., E. Wu, J.-C. Golaz, P. M. Caldwell, O. Watt-Meyer, S. K. Clark, J. McGibbon, G. Dresdner, K. Kashinath, B. Bonev, M. S. Pritchard, and C. S. Bretherton, 2024: Application of the

ACE Emulator to E3SMv2's global atmosphere model, with a focus on precipitation fidelity. *J. Geophys. Res.: Machine Learning and Comp.*, <https://doi.org/10.1029/2024JH000136>

Peter Caldwell. "AI Emulation of a Global Storm-Resolving Model." Presentation, Korean Institute for Science and Technology, Livermore, CA, Aug 20, 2024.

Peter Caldwell. "Update on AI for Earth System Modeling" Presentation, LLNL MFA Quarterly Discussion, Livermore CA, Oct 21, 2024.

Ullrich, P. A., Barnes, E. A., Collins, W. D., Dagon, K., Duan, S., Elms, J., et al. (2025). Recommendations for comprehensive and independent evaluation of machine learning-based Earth system models. *Journal of Geophysical Research: Machine Learning and Computation*, 2, e2024JH000496. <https://doi.org/10.1029/2024JH000496>

Elynn Wu, "E3SM All-Hands: AI/ML Emulation." Presentation, E3SM All-Hands Meeting, Denver, CO, Feb 27, 2025.

Donahue, A. S., E. Wu, W. A. Perkins, P. M. Caldwell, C. S. Bretherton, F. Rebassoo, J.-C. Golaz, 2025: Applying Corrective Machine Learning in the E3SM Atmosphere Model in C++. LLNL Tech. Report LLNL-TR-2002750

22-ERD-054: Data On Demand for Capable Space-Domain-Awareness Architecture

Project Overview

The growing complexity of space domain awareness (SDA) necessitates advanced modeling and simulation capabilities to address challenges in tracking, detecting, and analyzing objects across diverse orbital regimes. Current tools lack sufficient fidelity for modeling re-entry vehicles, cislunar dynamics, and EO/SWIR imaging signatures. Additionally, the ability to generate on-demand data pipelines for simulating realistic conflict scenarios is limited. This project aims to address these gaps by developing robust models, integrating them into existing frameworks, and conducting sensitivity analyses to identify critical parameters for SDA operations. These objects develop science and technology tools and capabilities to meet future national security challenges.

Telescopes and equipment were provided to produce images in optical and SWIR to measure sky background brightness at various times of day and weather. The observations informed the development of a software pipeline that includes the python package *Satellite Image Simulation Toolkit* (McGill, 2025) which can generate simulated images under varied sky conditions. *Space Situational Awareness for Python* (SSAPy; Yeager, 2022; Yeager, 2023b; Meyers, 2025) was developed with capabilities of orbital modeling from orbits in the Earth's atmosphere to cislunar space beyond the Moon. An open-source data set was produced using SSAPy and is made available on Lawrence Livermore National Laboratory's (LLNL) Green Data Oasis (Yeager, 2025). This data set has produced multiple publications and is a great resource for future research particularly in the areas of machine learning and statistical analysis related to cislunar orbits (Higgins, 2024, 2025a, 2025b). The project highlights commercial off-the-shelf (COTS) telescopes as a strong solution to many SSA architectures.

Mission Impact

The Data on Demand project supports LLNL in the Integrated Deterrence and Technology Competition Mission Focus Area and the High Performance Computing (HPC) Simulation, and Data Science Core Competency through systems analysis and the algorithmic war gaming of emerging deterrence challenges to identify/evaluate opportunities for prevailing in crisis. This project has produced deliverables exploring solutions to emerging security challenges associated with technology surprise in space, and other military domains. This research will provide equipment to continue related projects, and open-sourced data will be of use to the SDA TAP Lab and the development of future orbital machine learning models. The detection pipeline lines will also be shared and benefit future architecture studies. Commercial off-the-shelf (COTS) short-wave infrared sensors have been shown to cover the needs to track and detect luminous atmospheric sources and would be a great asset to an SSA architecture. Emerging threats require novel solutions, and this project has shown COTS telescopes as a viable, cheap, mobile solution for SSA and has developed science and technology tools and capabilities to meet future national security challenges. The procured equipment from this project will benefit LLNL's STARMOC.

Publications, Presentations, and Patents

Higgins, D., K. Pruett, T. Yeager, and M. Schneider. "SOM-erizing cislunar orbits: Classification of cislunar orbits using self-organizing maps (SOMs)." Poster presentation, Advanced Maui Optical and Space Surveillance (AMOS) Technologies Conference, September 2024.

<https://amostech.com/TechnicalPapers/2024/Poster/Higgins.pdf>.

Yeager, T., K. Pruett, and M. Schneider. "Long-term N-body stability in cislunar space." Poster presentation, Advanced Maui Optical and Space Surveillance (AMOS) Technologies Conference, September 2023a. <https://amostech.com/TechnicalPapers/2023/Poster/Yeager.pdf>.

Pruett, K., N. McNaughton, and M. Schneider. "Closely-spaced object classification using MuyGPyS." Poster presentation, Advanced Maui Optical and Space Surveillance (AMOS) Technologies Conference, September 2023.

<https://amostech.com/TechnicalPapers/2023/Poster/Pruett.pdf>.

Yeager, T., K. Pruett, and M. Schneider. "Unaided dynamical orbit stability in the cislunar regime." Poster presentation, Cislunar Security Conference, Johns Hopkins Applied Physics Laboratory, 2022.

Yeager, T., and K. Pruett. "Long-term N-body stability in cislunar space." Poster presentation, Advanced Maui Optical and Space Surveillance Technologies Conference, 2023b.

Pruett, K., N. McNaughton, and M. Schneider. "Closely-spaced object classification using MuyGPyS." Poster presentation, Advanced Maui Optical and Space Surveillance Technologies Conference, 2023.

"Exploring cislunar space via big datasets generated on HPC: Usefulness of SOMs for orbit prediction and statistics of cislunar families." Poster presentation, American Astronomical Society – Division on Dynamical Astronomy, 2025.

McNaughton, N., and K. Pruett. "Classifying closely spaced objects for space domain awareness." Oral presentation, LLNL DSSI Summer Slam, Livermore, CA, August 2023.

McNaughton, N., and K. Pruett. "Classifying closely spaced objects for space domain awareness." Poster presentation, LLNL ROTC Poster Symposium, August 2023.

Yeager, T. "SSAPy: A fast orbit simulation and SDA analysis code in Python – applied to the cislunar regime." Oral presentation, Space Domain Awareness Data Science Working Group, Sandia National Laboratories, NM, 2023c.

McNaughton, N., K. Pruett, and M. Schneider. "Classifying Closely Spaced Objects Using MuyGPs with Adversarial Noise." Poster presentation, LLNL ROTC Poster Symposium, Livermore, CA, August 2024.

22-ERD-056: Development of Advanced Terahertz Chiroptical Spectroscopy for Biological and Chemical Security

Project Overview

This project focused on the development of chiral metamaterials for terahertz (THz) beam polarization modulation, enabling the practical realization of THz circular dichroism (TCD) spectroscopy for rapid, reagent-free, high-sensitivity, and high-throughput chiral screening for drug discovery and the detection of biological and chemical threats. One of the primary drivers for this work is the current lack of birefringent optical crystals suitable for generating circularly polarized light in the THz frequency range. This limitation can be addressed by designing artificial subwavelength metamaterials. By developing such metamaterials, we can facilitate new types of chiroptical spectroscopy—specifically, TCD spectroscopy—which hold significant promise for biomedical technology, as well as biological and chemical security applications.

In this project, we have developed two different types of metamaterials: 1) Microfabricated, reconfigurable chiral kirigami metamaterials, 2) 3D-printed helical meta-arrays exhibiting chiral metahologram properties. Additionally, we have demonstrated TCD spectroscopy using femtosecond lasers for the detection of (i) chiral metal–amino acid nanostructures and (ii) controlled substances such as fentanyl and explosives. These results highlight the direct potential of this technology for biomedical applications and national security. Both THz and TCD spectroscopy offer X-ray-like penetration depths combined with the molecular recognition capabilities of Raman or infrared spectroscopy, opening up new possibilities across a range of technologies.

Mission Impact

The development of chiral metamaterials and TCD spectroscopy advances the fundamental understanding of light–matter interactions in laser and optical physics, as well as asymmetric molecular assembly and biochemical reactions. These technologies also have practical applications in the detection and mitigation of high explosives and controlled substances such as fentanyl, addressing threats across the entire spectrum. As a result, this work is expected to directly enhance the security and resilience of the nation and its critical infrastructure against chemical, biological, and natural hazards. Furthermore, it enables the National Nuclear Security Administration (NNSA) to develop new strategies for responding to emerging national security challenges.

Publications

Choi, Wonjin, Sang Hyun, Minjeong Cha, and Nicholas Kotov. 2024. "Chiral Kirigami for Bend-Tolerant Reconfigurable Hologram with Continuously Variable Chirality Measures." *Advanced Materials*. <https://doi.org/10.1002/adma.202401131>. LLNL-JRNL-845947.

Chae, Soosang, Wonjin Choi, Lisa Nebel, Chang Hee, Quinn Besford, André Knapp, Pavlo Makushko, Yevhen Zabala, Oleksandr Pylypovskyi, Min Woo, Stanislav Avdoshenko, Oliver Sander, Denys Makarov, Yoon Jang, Andreas Fery, Jin Young, and Taeil Lee. 2024. "Kinetically

controlled metal-elastomer nanophases for environmentally resilient stretchable electronics." *Nature Communications*. <https://doi.org/10.1038/s41467-024-47223-6>. LLNL-JRNL-845946.

Choi, Wonjin, Michael Armstrong, Jae Hyuck, and Taeil Lee. 2024. "Toward high-power terahertz radiation sources based on ultrafast lasers." *Journal of Materials Chemistry C*. <https://doi.org/10.1039/D4TC01502A>. LLNL-JRNL-862523.

Kwon, Junyoung, Jaebum Jeon, Mingu Lee, Serin Jeong, Wonjin Choi, Kyungmin Kim, and Jihyeon Yeom. 2025. "Enantioselective Se lattices for stable chiroptoelectronic processing media." *Nature Communications*. <https://doi.org/10.1038/s41467-025-59091-9>. LLNL-JRNL-2005356.

Choi, Wonjin, Ji-Young Kim, Myonghoo Hwang, Chungman Lim, Bumchul Park, Ahmet Emre, Sanghyun Lee, and Nicholas Kotov. 2025. "Highly Elliptic Circular Dichroism of Copper Aspartate One-Dimensional Nanostructures across the Ultraviolet to Terahertz Ranges." *Nano Letters*. <https://doi.org/10.1021/acs.nanolett.5c00411>. LLNL-JRNL-872303.

Choi, Wonjin, Changhee Cho, Deuk-Kyu Hwang, and Taeil Lee. 2023. "Kirigami Photopiezo Catalysts for Self-Sustainable Environment Remediation." *ACS Nano*. <https://doi.org/10.1021/acsnano.3c05787>. LLNL-JRNL-845604.

Chae, Soosang, Wonjin Choi, Su-Hyeong Lee, Quinn Besford, and Andreas Fery. 2025. "Tunneling Barrier-Integrated Gold Nanofilms for Negative Strain Gauging with Near-Zero Energy Consumption." *Nano Letters*. <https://doi.org/10.1021/acs.nanolett.4c06365>. LLNL-JRNL-871474.

Records of Invention

Choi, Wonjin, Mike Armstrong, Songyun Gu, Widi Moestopo, and Xiaoxing Xia. 2025. "Encrypted Chiral Holograms using Helical Photonic Metamaterials." 2025-221.

Choi, Wonjin, Changhee Cho, and Taeil Lee. 2023. "Kirigami photo-piezo catalysts for self-sustainable environment remediation." IL-13895.

23-ERD-003: High Resolution Chronology of the Solar System

Project Overview

High precision chronometry of planetary materials is essential for addressing key questions about the origin and evolution of the Solar System and the processes of planet formation. At present, only a single laboratory worldwide routinely applies the U Pb chronometer at the highest level for such measurements, which is not sufficient to resolve the growing number of questions in this rapidly advancing field. The overarching goal of this project was to establish the U Pb chronometric system at LLNL and to sustain LLNL as a leading planetary chronology center in the United States.

The U Pb isotopic system represents the pinnacle of isotope dilution mass spectrometry. It requires the analysis of extremely small quantities of U and Pb (typically less than 100 pg) and is highly susceptible to contamination, which demands exceptional analytical rigor. To perform U Pb chronometry at the current state of the art, we needed to obtain a unique isotopic tracer that contains certified quantities of ^{233}U , ^{235}U , ^{202}Pb , and ^{205}Pb . This tracer is unique because it contains the exceedingly rare ^{202}Pb isotope, is exceptionally well calibrated, and is supported by thoroughly vetted data reduction software.

A key objective of this LDRD was to obtain the EARTHTIME ET2535 tracer for use at LLNL. Access to this tracer required an intensive accreditation process administered by the EARTHTIME initiative, as it is only distributed to laboratories that demonstrate the capability to exploit its full precision and accuracy.

In parallel, we applied our developing capabilities to frontier problems in cosmochemistry. We conducted research on early Solar System evolution, as well as on the formation and early evolution of the Moon and Mars, using U Pb chronometry to provide high precision age constraints on key planetary materials.

Mission Impact

This project supported both mission focus areas and the laboratory's enduring core competencies. The work conducted under this proposal advanced the development of existing and new isotope analysis techniques that are directly relevant to programmatic R&D efforts within our team. This project strengthened the Nuclear, Chemical, and Isotope Science and Technology core competency, as well as the Earth and Atmospheric Science core competency. The isotope analysis and radiometric capabilities used across program areas at LLNL rely on the technical foundations established by cosmochemical research on planetary materials. Many of the techniques developed for cosmochemistry are readily transferable to programmatic research. The need to remain competitive in cosmochemistry, by producing state of the art data on very small samples with low abundances of key elements and subtle isotopic and geochemical signatures, provides LLNL scientists with significant advantages over those working solely with anthropogenic signatures. These capabilities enable more sensitive, precise, and reliable isotopic measurements across a wide range of applications. The scientific outcomes of this LDRD have already helped secure NASA funding for basic research and will support future NASA funding opportunities associated with upcoming sample return missions, including the Artemis program. Collectively, the scientific results

and analytical capabilities developed through this grant have enabled LLNL to maintain and strengthen its leadership role in isotopic signature science and in space and planetary research.

Publications, Presentations, and Patents

Borg L. E., Kruijjer T. S., Liu M.-C., Roberts A. G., Wimpenny J., Maina O. N. Z., Boro J., Shearer C. K. and Samperton K. M. (2025) Temporal relationships among lunar crustal rocks. *Geochimica et Cosmochimica Acta* 410, 266–280. LLNL-JRNL-2011687.

Schönbächler M., Bouvier A., Kita N.T., Kruijjer T.S. (2025) Initial Conditions of Planet Formation: Time Constraints from Small Bodies and the Lifetime of Reservoirs in the Solar Protoplanetary Disk. *Space Science Reviews, Space Sci Rev* 221, 97 (2025). LLNL-JRNL-2005397-

Grewal, D. S., Zhang, Z., Manilal, V., Kruijjer, T. S., Bottke, W. F., & Stewart, S. T. (2025). Protracted core formation and impact disruptions shaped the earliest outer Solar System planetesimals. *Science Advances*, 11(40), eadw1668. LLNL-JRNL-2005388

Barnes J.J., Nguyen A.N. (...) Kruijjer T.S. (and 84 other co-authors) (2025) The variety and origin of materials accreted by Bennu's parent asteroid. *Nature Astronomy*, <https://doi.org/10.1038/s41550-025-02631-6>.

Kruijjer, T.S., Borg, L.E., Render, J., Brennecka, G.A., Wimpenny, J., Shearer, C.K., Agee, C.B. (2025) Isotopic constraints on the origin of a differentiated achondrite from Hassi El Madani 002. Lunar and Planetary Science Conference #1130, The Woodlands, TX, USA.

Borg, L., Kruijjer, T., Liu, M., Roberts, A., Maina, O., Wimpenny, J., Boro, J., Shearer, C., Samperton, K. (2025) Temporally compressed crustal magmatism on the lunar nearside. Lunar and Planetary Science Conference #1024, The Woodlands, TX, USA.

Goss, K.R., Borg, L.E., Kruijjer, T.S., Liu, M.C., Crow, C.A., Brearley, A.J., Shearer, C.K. (2025) Correlated microstructural and chronometric studies of lunar zircons: Interpreting zircon ages from lunar breccia 14321. Lunar and Planetary Science Conference #2483, The Woodlands, TX, USA.

Shearer, C.K., Simon, S.B., Setera, J.B., Simon, J., Spilde, M., Borg, L.E., Kruijjer, T.S., Yen, C.J.-K., Jolliff, B.L. (2025) Mg-suite volcanics: A magmatic or impact origin? Lunar and Planetary Science Conference #1320, The Woodlands, TX, USA.

Spitzer F., Burkhardt C., Kruijjer T.S., Kleine T. (2025) Comparison of the earliest NC and CC planetesimals: Evidence from ungrouped iron meteorites. *Geochimica et Cosmochimica Acta* 397, 134-148. LLNL-JRNL-870730

Borg L. E. and Kruijjer T. S. (2025) A tale of two planets: Disparate evolutionary models for Mars inferred from radiogenic isotope compositions of Martian meteorites. *Proc. Natl. Acad.*

Sci. U. S. A (PNAS). 122, e2404257121. LLNL-JRNL-861035.

Kruijjer, T. S., Borg, L. E., Render, J., Brennecka, G. A., Wimpenny, J., Shearer, C. K., & Agee, C. B. (2025). Isotopic Constraints on the Origin of a Differentiated Achondrite from Hassi el Madani 002. LPI Contributions, 3090, 1130

Borg, L. E., Kruijjer, T. S., Liu, M. -C., Roberts, A. G., Maina, O. N. Z., Wimpenny, J., Shearer, C. K., & Samperton, K. (2025). Temporally Compressed Crustal Magmatism on the Lunar Nearside. 56th Lunar and Planetary Science Conference, Abstract #1024.

Kruijjer T.S., Borg L.E., Udry A., Filiberto J. (2024) Formation and interior evolution of Mars. *Treatise on Geochemistry* 3rd edition, 7, 481-520. Doi: 10.1016/B978-0-323-99762-1.00113-3. LLNL-JRNL-853697

Kruijjer T. S., Borg L. E., Cassata W. S., Wimpenny J., Brennecka G. Shearer C. K., and Simon S. B. "Chronology of alkali anorthosite 14304 clast "b" records basin forming impact at ~3.95 Ga". *Geochimica et Cosmochimica Acta* 358, 61-76(2023) LLNL-JRNL-844335.

Borg L. E. and Carlson, R. W. "The Evolving Chronology of Moon Formation". *Annual Review of Earth and Planetary Sciences*, 51 (2023) LLNL-JRNL-832455.

Render, J, Wimpenny J., and Borg L. "Gallium isotopic constraints for the origin of the Earth Moon system". *Earth and Planetary Science Letters* 661, 118146 (2023). LLNL-JRNL837296.

Borg L. E., Gaffney A. M. "A deep lunar magma ocean" Annual Meeting of the Meteoritical Society Meeting. UCLA, Los Angeles, CA, USA. LLNL-ABS-849749

Kruijjer T. S, Burkhardt C., Borg L. E., Kleine T. (2023) Isotopic and Chronological Evidence for an Impact Origin of Pallasites. Annual Meeting of the Meteoritical Society Meeting, UCLA, Los Angeles, CA, USA.

Kruijjer T. S. Tungsten isotopes and the early Solar System" (2023) Abstract EGU General Assembly LLNL-CONF-847653

Render, J, Wimpenny J., and Borg L "Implications for the origin of the Earth-Moon system from gallium isotopes" Abstract Lunar and Planetary Science Conference #2457 (2023).

Borg L. E., Brennecka G. A., Kruijjer T. S. The origin of volatile element depletion in the EarthMoon system" Abstract Lunar and Planetary Science Conference # 1054. (2023) LLNLPRES-847657

Borg L. E. "Science objectives enabled by the Endurance mission" Abstract Endurance Science Workshop (2023) LLNL-ABS-850956

23-ERD-004: Nuclear Experiments from Lattice Quantum Chromodynamics Supercomputing Simulations

Project Overview

We integrated numerical simulations of Quantum Chromodynamics (QCD), the underlying theory of nuclear physics, with existing experimental data and with our highest precision nuclear theories. We were able to provide, for the first time, constraints on the most poorly determined features of our microscopic nuclear reaction models to enable a more robust prediction and evaluation of light ion reactions. This is a new strategic capability that gives high-precision access to quantities that are otherwise very difficult to determine experimentally. This launches a new era of LLNL nuclear evaluation and reactions derived from QCD and a deeper understanding of our cosmos. We simulated QCD and extracted the relevant scattering cross sections (pion-nucleon and nucleon-nucleon) using the method of Lattice Gauge Theory (LQCD) on the fastest LLNL supercomputers (Lassen, early access El Capitan and Tuolumne). We developed the tools to integrate these results with existing experimental data and calculated the corresponding low energy constants (LEC) of the resulting Effective Field Theory (EFT). These are the essential inputs to ab-initio nuclear theory computations of reaction rates of light ions. We found that the inclusion of LQCD numerical results significantly improves the accuracy of the LECs demonstrating that our method is of significant value to LLNL and should be part of the LLNL nuclear evaluation and reactions workflow. This was the overarching goal of this research and has now been demonstrated. The developed tools are highly sophisticated and the result of exhaustive analysis of the LQCD results and existing experimental data.

Mission Impact

This research supports NNSA's mission by developing science and technology tools and capabilities to meet future national security challenges and address some of DOE's energy and environmental security missions. Nuclear, Chemical, and Isotopic Science and Technology / Physics at the frontier: This effort solidified the LQCD integration with experimental data and ab initio nuclear theory and provided better error sizes for pion-nucleon and nucleon-nucleon interactions. This is of direct interest to LLNL's nuclear data. Stockpile Science: Stockpile Science needs accurate nuclear reaction data with quantifiable uncertainties. Improved predictions of light-ion reactions enabled by this work are important inputs to Stockpile Science. We made our science software highly performant on the new exascale hardware and entered the 2025 Gordon Bell Prize competition. Basic Science: The pion-nucleon and nucleon-nucleon interactions are at the core of many nuclear physics processes. They are part of the lifecycle of stars as they ignite and eventually burn their nuclear fuel. They are part of our understanding of fusion and of the evolution of our cosmos from the Big Bang to today as they play a crucial role in the making of nucleons. Therefore, the results of this research are far reaching and are of interest to a wide audience.

Publications, Presentations, Patents

Aaron, Meyer. 2024. "Connecting Lattice QCD Nucleon-Pion Scattering to Nuclear Ab Initio Calculations." *American Physical Society April Meeting*. Sacramento, CA.

Aaron, Meyer, and al et. 2024. "Stealth dark matter spectrum using LapH and Irreps." *Physical Review D* 110 (095001).

2024. "Connecting Lattice QCD Nucleon-Pion Scattering to Nuclear Ab Initio Calculations." *The 41st International Symposium on Lattice Field Theory (Lattice 2024)*. Liverpool, United Kingdom.

Sungwoo, Park. 2024. "Lattice QCD and Supercomputing for Nuclear Physics." *International Conference on Nuclear Theory in the Supercomputing Era - 2024(NTSE-2024)*. Busan, South Korea.

23-ERD-005: Multifunctional Hohlraums

Project Overview

Advances in inertial confinement fusion (ICF) depend on improved laser target design. The hohlraum converts laser energy into X-rays that drive fuel implosion. Using “cocktail” alloys enhances hohlraum X-ray drive by increasing wall opacity and reducing energy loss. Over the three-year project, simulations of more than 10 million heavy-metal alloys using the analytical model of Hammer and Rosen (Phys. Plasmas 10, 2003) coupled with machine-learning optimization in LLNL’s Materials Acceleration Platform, and validated with Lasnex radiation-hydrodynamics simulations, predicted that Ta₁₀W₁₀Au₁₀Bi₇₀ outperforms Au hohlraums by 10% and Bi hohlraums by 4% in X-ray flux. Systematic studies of deposition parameters including mode, pressure, temperature, and substrate tilt angle enabled the fabrication of >50 μm-thick Ta₁₀W₁₀Au₁₀Bi₇₀ coatings with high electrical resistivity, low oxygen content.

Mission Impact

This project supports the ICF program goal to advance high energy density (HED) experiments and ICF yield. We developed and demonstrated a novel Ta₁₀W₁₀Au₁₀Bi₇₀ high-entropy alloy for next-generation ICF hohlraums. This hohlraum can be used in future HED and ICF experiments, including magnetically assisted ICF implosions, and could potentially increase fusion energy yield at the National Ignition Facility (NIF). The project also strengthened the Laboratory’s Core Competency in Advanced Materials and Manufacturing.

Publications, Presentations, and Patents

Bayu Aji, L. B. "HIPIMS deposition of ultrathick Au-Ta coatings: effects of deposition rate and substrate tilt." ICMCTF, San Diego, CA, May 21, 2023. LLNL-PRES-849481.

Bayu Aji, L. B. "High entropy alloys coatings for inertial confinement fusion hohlraums." ICMCTF, San Diego, CA, May 11, 2025. LLNL-PRES-2005408.

Bocklund, B. J., et al. 2025. "Calphad modeling of Bi-Pt supported by first-principles calculations." LLNL. LLNL-JRNL-2011983-DRAFT.

Goodelman, D. C. "A combinatorial approach to developing sputter deposited AuBiTaW high-entropy alloy films for inertial confinement fusion applications." PowerPoint, ICMCTF, San Diego, CA, May 19, 2024. LLNL-PRES-864507.

Goodelman, D. C. "High entropy alloys for next-generation hohlraums." PowerPoint, 25th Target Fabrication Specialists Meeting, San Diego, CA, August 25, 2024. LLNL-PRES-866974.

Goodelman, D. C., et al. 2025a. *Combinatorial deposition of ultrathick Ta-W-Au-Bi high entropy alloys for next-generation hohlraums by DCMS*. LLNL. LLNL-JRNL-871503.

Goodelman, D. C., et al. 2025b. "High-rate deposition of ultrathick bismuth films by direct-current magnetron sputtering." *Vacuum* 239: 114385. <https://doi.org/10.1016/j.vacuum.2025.114385>.

Goodelman, D. C., et al. 2025c. *Sputter deposition of Bi films onto rotating substrates for inertial confinement fusion targets*. LLNL. LLNL-JRNL-2008214.

Goodelman, D.C., et al. 2025d. "Combinatorial deposition of Au-Bi alloy films via high-rate, direct-current magnetron sputtering for next-generation hohlraums". LLNL. LLNL-JRNL-2011017.

Goodelman, D.C., et al. 2025e. "Direct-current magnetron sputter deposition of TaW₁₀AuBi high entropy alloys for inertial confinement fusion applications". LLNL. LLNL-JRNL-2011343-DRAFT.

Goodelman, D. C. "Sputter deposition of Ta-W-Au-Bi high entropy alloys for inertial confinement fusion hohlraums." PowerPoint, ICMCTF, San Diego, CA, May 11, 2025.

Kim, E., et al. 2024. "Effects of growth rate and dynamic substrate tilt on properties of Au-Ta alloy films deposited by HiPIMS." *Surf. Coat. Technol.* 493: 131231.
<https://doi.org/10.1016/j.surfcoat.2024.131231>.

Kim, E. "Combinatorial approach to develop sputter-deposited high-entropy alloy films for inertial confinement fusion applications." PowerPoint, TMS Annual Meeting & Exhibition, Orlando, FL, March 3, 2024. LLNL-CFPRES-2011473.

Strozzi, D. J. "Novel high-entropy alloys for inertial fusion hohlraums." PowerPoint, 66th Annual Meeting of the APS Division of Plasma Physics, Atlanta, GA, October 7, 2024. LLNL-CONF-869994.

Strozzi, D. J., et al. 2025. "Increased inertial fusion X-ray drive with high-entropy alloy hohlraums." LLNL. RR0094769.

Vishnoi, N., et al. 2024. *Sputter deposition of Ta₁₀W₁₀Au₁₀Bi₇₀ films for next generation hohlraums*. LLNL. LLNL-TR-867948. <https://doi.org/10.2172/2427480>.

23-ERD-006: Understanding Spectral Dependence of Laser-induced Damage Precursors in Dielectric Materials

Project Overview

High peak and average power laser systems are typically limited by the handling fluence of the optical components. In particular, the multilayer dielectric coatings are known to be much lower operational fluence than the more ideal bulk materials. In this project we proposed and succeeded in probing different established classes of damage prone precursors at different wavelengths to understand their fundamental laser damage response as a function of wavelength. This study helped to shed light on the fundamental physics of the non-linear precursors that govern laser damage phenomena for ns-regime pulsed laser damage. In this study, we utilized the onsite coating capabilities to purposefully generate laser damage-prone precursors in hafnia-based coatings (both single and multi-layer coatings). Specifically, we engineered coatings with craze lines initiated by nodules, generated coatings with our xenon-based coating process to suppress nanobubble formation and generated hafnia coatings under controlled oxygen flow conditions to study hafnia sub-oxides and oxygen flow dependence. In these studies we found that craze lines are rife with precursors that are sensitive to ultra-violet light but not to infrared light; we found that the removal of nanobubbles helps with all wavelengths tested, but is most impactful for ultra-violet light; we also found that ultra-violet laser damage performance of hafnia is closely matched to oxygen flow rate, while the infrared performance may be slightly better at lower flow rates.

During this LDRD project we also successfully implemented a new laser damage testing capability, namely a wavelength agile damage test station to study the spectral response of known laser-induced damage precursors. This is a unique and important capability for Lawrence Livermore National Lab, allowing us to understand the spectral response of materials under high intensity irradiation and damage. This is a vital tool to understand non-linear optical response at wavelengths that we have previously been unable to test at.

Mission Impact

This project has had a significant mission impact by advancing our understanding of optical coating defects through groundbreaking research that has been widely recognized in numerous high-impact journals and through invited oral presentations at international conferences. The outcomes of this work directly support critical programmatic efforts, including National Ignition Facility (NIF), Matter in Extreme Conditions (MEC), High-Repetition-Rate Advanced Petawatt Laser System (HAPLS), Department of Defense (DOD), and Atomic Vapor Laser Isotope Separation (AVLIS), strengthening their scientific and technical foundations. Furthermore, the successful stand-up and qualification of a new wavelength-agile damage test station now provides unique capability to investigate the spectral response of laser-induced damage precursors, enhancing our ability to predict and mitigate risks in high-power laser systems.

Publications

Suratwala, Tayyab, C. Wren Carr, Christopher Stolz, *Optic Technologies Enabling Fusion Ignition*, New Jersey, 2025.

Harthcock, Colin, Amira Guediche, Saaxewer Diop, Christopher J Stolz, Raluca A Negres, Gener Gatmaitan, Rebeca I Rangel, *et al.* "Laser Damage of Crazed Electron-Beam High-Reflectors Following Infrared and Ultraviolet Irradiation in the Nanosecond Pulse Regime." *Applied Optics* 64, no. 25 (2025): 7457-64.

Harthcock, Colin, Hoang Nguyen, Devika Vipin, Mengbeng Huang, "The impact of high-temperature annealing on hafnia-silica composite coatings deposited via ion beam sputtering for high-peak power 1064 nm lasers" *Optical Materials Express*, Accepted.

Oral Presentations

Harthcock, Colin, Christopher J Stolz. "Improvements to multilayer dielectric coatings to enable inertial confinement fusion at the National Ignition Facility (NIF)" Invited talk, International Conference on Metallurgical Coatings and Thin Films, San Diego, CA, May 20, 2024.

Harthcock, Colin, Amira Guediche, Saaxewer Diop, Jungmin Ha, S. Roger Qiu, Paul B. Mirkarimi, Thomas Voisin, Christopher A. Colla, Harris E. Mason, Raluca A. Negres, Gabe Guss, Devika Vipin, Mengbing Huang. "The Impact of Nano-Bubbles on Laser Damage Performance of IBS Fabricated MLD Coatings" Invited talk, Optical Interference Coatings Conference, Tuscan, AZ, May 22, 2025.

Diop, Saaxewer, Gener Gatmaitan, Christopher J. Stolz, Colin Harthcock, Amira Guediche, Eyal Feigenbaum, Tsion Teklemariam, Matt Brophy "High fluence oblique multilayer high reflecting coating with minimal differential phase angle over a wide angular or spectral range" SPIE Laser Damage, San Ramon, CA, October 5, 2024.

Guediche, Amira, Saaxewer Diop, Jae Hyuck Yoo, Gener D. Gatmaitan, Raluca Negres, Ryan Gini, Warren L. York, Tian Li, Colin Harthcock "Understanding the wavelength dependent laser damage response for nanobubbles in ion beam sputtered hafnia layers" SPIE Laser Damage, San Ramon, CA, October 5, 2024.

Guediche, Amira, Michel Arrigoni, Francesco Delloro, Serge Guetta, Nathan Menetrier, Laurent Belliard, Bernard Perrin, Marc Duquennoy, Emilien Lescoute, Michel Boustie, Hervé Piombini "Mitigating laser-induced damage and plasma-induced shock waves in optical components with a coating solution for high-power laser applications" SPIE High-Power Laser Ablation VIII, Santa Fe, NM, February 29 2024.

Guediche, Amira, Saaxewer Diop, Raluca Negres, L. B. Bayu Aji, and Colin Harthcock "Influence of Oxygen Flow and Sub-Stoichiometry on the Optical and Damage Resistance Properties of Hafnium Oxide Thin Films" Optical Interference Coatings Conference, Tuscan, AZ, May 22, 2025.

23-ERD-007: Addressing Key Physics Problems in High-Energy-Density Plasmas with a Novel Kinetic Simulation Capability

Project Overview

Many important physical processes in inertial confinement fusion (ICF) and dense Z-pinch (DZP) experiments require a kinetic (velocity-space-dependent) description. Conventional particle-in-cell (PIC) methods are poorly suited for high-energy-density (HED) plasmas, due to restrictive time-step constraints and the inability to conserve energy. In a previous LDRD (21-FS-048), we demonstrated that a fully implicit PIC formulation overcomes these limitations: it conserves energy even when coupled with Coulomb collision models and can be solved efficiently with large grid cells and large time steps. Thus, it is feasible to use this method to study kinetic effects in ICF and DZP plasmas on hydro-like time and spatial scales. In this follow-on LDRD, we advanced this methodology into a high-fidelity tool for production-scale simulations and used it to answer key questions relevant to ICF and DZP experiment.

The fully implicit collisional PIC algorithm was implemented in the prototype code PICNIC, written in C++ and supporting 1D/2D planar, 1D/2D/axisymmetric cylindrical, and 1D axisymmetric spherical geometries. Under this project, we developed the axisymmetric cylindrical and spherical geometries needed for DZP and ICF simulations, respectively. Using PICNIC, we reproduced experimental trends of the measured neutron yield in DZP, including contributions from non-local beam-target fusion. For ICF plasmas, we investigated key open questions – for example, the role of electron viscosity in plasma shock heating, and whether non-local effects explain anomalous neutron spectra measured in burning plasma shots at the National Ignition Facility (NIF). Finally, we made significant progress porting PICNIC's algorithms into the exascale PIC code WarpX. This effort continues under the DOE KISMET SciDAC project, where WarpX is being applied to kinetic studies of inertial fusion energy (IFE) plasmas.

Mission Impact

This research produced a new kinetic simulation capability for studying HED plasmas, directly advancing the LLNL/NNSA mission to develop science and technology tools and capabilities to meet future national security challenges. By implementing the algorithm into the WarpX code, the project enables LLNL to fully leverage new exascale systems such as El Capitan and Tuolumne for large-scale kinetic plasma studies. The methods developed are also central to the LBL-led KISMET DOE SciDAC project – the first SciDAC awarded for inertial fusion energy (IFE) studies – in which LLNL is a key partner, thereby strengthening DOE/NNSA collaborations and broadening the impact across federal research programs.

Publications

Angus, Justin, William Farmer, Alex Friedman, Debojyoti Ghosh, Dave Grote, David Larson, and Anthony Link. 2023. "An implicit particle code with exact energy and charge conservation for

electromagnetic studies of dense plasmas." *Journal of Computational Physics* 491, no. 112383 (July): <https://doi.org/10.1016/j.jcp.2023.112383>. LLNL-JRNL-845634.

Angus, Justin, Yichen Fu, Vasily Geyko, Dave Grote, and David Larson. 2025. "Moment-preserving Monte-Carlo Coulomb collision method for particle codes." *Journal of Computational Physics* 531, no. 113927 (March): <https://doi.org/10.1016/j.jcp.2025.113927>. LLNL-JRNL-867233.

Angus, Justin, William Farmer, Alex Friedman, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, and Anthony Link. 2024. "An implicit particle code with exact energy and charge conservation for studies of dense plasmas in axisymmetric geometries." *Journal of Computational Physics* 519, no. 113427 (September): <https://doi.org/10.1016/j.jcp.2024.113427>. LLNL-JRNL-862393.

Fu, Yichen, Justin Angus, Hong Qin, and Vasily Geyko. 2025. "Energy-momentum-conserving stochastic differential equations and algorithms for the nonlinear Landau-Fokker-Planck equation." *Physical Review E* 111, no. 025211 (February): <https://doi.org/10.1103/physreve.111.025211>. LLNL-JRNL-870465.

van de Wetering, Johannes Johgan, Justin Ray Angus, William Farmer, Vasily Geyko, Debojyoti Ghosh, Dave Grote, Chris Weber, and George Zimmerman. 2025. "Particle-in-Cell Simulations of Burning ICF Capsule Implosions." *Physical Review E* <https://link.aps.org/doi/10.1103/zwjx-jbxl>. LLNL-JRNL-2006642.

Angus, Justin, Johannes Johgan van de Wetering. 2025. "A Monte-Carlo Method for Coulomb Collisions in Moderately Coupled Plasmas." *Journal of Computational Physics*. (accepted) LLNL-JRNL-2003045.

Angus, Justin Ray, Jinyuan Dun, William Farmer, Vasily Geyko, Dave Grote, David Larson, Johannes Johgan van de Wetering, George Zimmerman. 2025. "Kinetic study of strong shock waves in fully ionized plasmas." *Physical Review E* (pending minor edits) LLNL-JRNL-2005839.

Posters

Angus, Justin, William Farmer, Alex Friedman, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, and Anthony Link. 2023. "An implicit particle code with exact energy and charge conservation for electromagnetic studies of dense plasmas." (Poster Presentation at APS Division of Plasma Physics, Denver, CO, November). LLNL-POST-855875.

Angus, Justin, Johannes van de Wetering, William Farmer, Alex Friedman, Yichen Fu, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, and George Zimmerman. 2025. "An implicit particle code for fully kinetic simulations of burning plasmas." (Poster Presentation at IFE-STAR Conference, Breckenridge, CO, April). LLNL-POST-2004062.

Angus, Justin, William Farmer, Alex Friedman, Debojyoti Ghosh, Dave Grote, David Larson, and Anthony Link. 2023. "An implicit particle code with exact energy and charge conservation for electromagnetic studies of dense plasmas." (Poster Presentation at IEEE International Conference on Plasmas Science, Santa Fe, NM, May). LLNL-POST-848824.

Dun, Jinyuan, Justin Angus, William Farmer, Alex Friedman, Vasily Geyko, Debojyoti Ghosh, Frank Graziani, Dave Grote, David Larson, Anthony Link, George Zimmerman, and S Fujioka. 2023. "Particle-in-cell Simulations of Shocks in Plasmas." (Poster Presentation at 65th Annual Meeting of the APS Division of Plasma Physics, Denver, CO, November). LLNL-POST-855813.

Vasily Geyko, Justin Angus, 2024, "Kinetic study of dynamic Z-pinch with an energy-conservative particle code." (Presented at 66th Annual Meeting of the APS Division of Plasma Physics, Atlanta, GA, October 2024).

Presentations

Justin Angus, William Farmer, Alex Friedman, Yichen Fu, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Anthony Link, Joshua Ludwig, George Zimmerman, Jinyuan Dun, 2024, "A fully implicit particle code for dynamically compressing plasmas: Solver implementation and initial applications." (Presented at Monthly Joint Japan-US Seminar Series on HEDS, webex, May 2024).

Justin Angus, William Farmer, Alex Friedman, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Anthony Link, 2024, "A fully implicit particle code for dynamically compressing plasmas: Solver scaling and performance." (Presented at 18th Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, April 2024).

Justin Angus, Johannes van de Wetering, 2025, "A binary collision method for screened Coulomb collisions in moderately coupled plasmas." (Presented at Seminar at Imperial College, London, Imperial College, London, June 2025).

Justin Angus, William Farmer, Alex Friedman, Yichen Fu, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Anthony Link, Joshua Ludwig, Johannes van de Wetering, George Zimmerman, 2024, "A fully implicit particle code for dynamically compressing plasmas: solver implementation and initial applications." (Presented at IFE Seminar series, LLNL, October 2024).

Justin Angus, William Farmer, Alex Friedman, Yichen Fu, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Anthony Link, Johannes van de Wetering, George Zimmerman, 2025, "An implicit particle code for kinetic simulations of dynamically compressing plasmas." (Presented at 2025 IEEE Pulsed Power & Plasmas Science Conference, Berlin, Germany, June 2025).

Justin Angus, 2025, "High-performance collisional implicit particle-in-cell methods for fully kinetic simulations of dynamically compressing plasmas." (Invited talk, to be presented at The International Conference on Numerical Simulation of Plasmas, Irvine, CA, November 2025).

Johannes van de Wetering, Justin Angus, William Farmer, Alex Friedman, Yichen Fu, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Anthony Link, Josh Ludwig, George Zimmerman, 2025, "Kinetic study of alpha knock-on RIFs with an energy-conserving particle-in-cell code." (Presented at Neutron Reaction-in-Flight (RIF) Workshop, LLNL, March 2025).

Johannes van de Wetering, Justin Angus, William Farmer, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Chris Weber, George Zimmerman, 2025, "Particle-in-cell simulations of burning capsule implosions." (Presented at 67th Annual Meeting of the APS Division of Plasma Physics, Long Beach, CA, November 2025).

Johannes van de Wetering, Justin Angus, William Farmer, Vasily Geyko, Debojyoti Ghosh, Dave Grote, David Larson, Chris Weber, George Zimmerman, 2025, "Particle-in-cell simulations of burning capsule implosions." (Presented at Anomalous Absorption Conference, Sedona, AZ, March 2025).

Code

Angus, Justin, and Debojyoti Ghosh. 2024. *PICNIC*. <https://github.com/JustinRayAngus/PICNIC>.

23-ERD-008: Laser-Induced Desorption and Redeposition in Fused Silica

Project Overview

The motivation for this research was to address a newly observed laser-induced damage mechanism in fused silica optics, which poses a challenge to large-aperture laser systems such as the National Ignition Facility (NIF) at higher fluences. Previous studies indicated that non-damaging exposure of fused silica surfaces to 351-nm laser pulses above approximately 12 J/cm^2 leads to a substantial increase in laser-induced damage density during subsequent exposures above approximately 18 J/cm^2 . This phenomenon could limit the ability of large-aperture laser systems to achieve higher energy densities, despite advances in conventional damage mitigation techniques.

Results demonstrated that annealed samples, particularly those treated in vacuum, exhibited significantly reduced degradation rates, implicating nonbridging oxygen hole centers (NBOHCs) as the primary absorbing defects. Environmental control experiments revealed that increased gas pressure, especially with oxygen, inhibited the degradation effect, suggesting that both precursor oxidation and reduced transport contribute to mitigation.

Mission Impact

This work both explains and demonstrates remedies to a next-generation laser-induced damage mechanism, helping maintain leadership in the development of next-generation lasers and optics. Understanding of laser-induced desorption and redeposition directly supports inertial confinement fusion energy and hence the High Energy Density Science Core Competency. The successful completion of this project directly supports the Optics, Optics Manufacturing Technologies, and Laser-Material Interaction (LMI) Science R&D priorities within the Lasers and Optical Science and Technology Core Competency.

Presentations

Taylor, L., D. Cross, C. Miller, A. Eshun, S. Diop, K. Sasan, M. Norton, M. O'Brien, S. Gorman, A. Newhouse, W. Hollingsworth, J. Eggen, R. Plummer, C. Carr "Impact of ambient conditions on laser induced damage precursors generation." Presentation at SPIE Conference October 7-10, 2024., San Ramon, CA,

23-ERD-009: Advanced In-situ Processes Monitoring Diagnostics and Ex-situ Material Characterization for Laser-based Metal Additive Manufacturing Processes

Project Overview

There is need for on-machine in-situ process characterization for laser-based advanced manufacturing processes and ex-situ post fabrication qualification of the produced parts. Here our goal was to advance a recently demonstrated in-situ ultrasound technique for interrogating laser melt pools, propose a novel in-situ arrayed eddy current diagnostic for full field thermal measurements, and investigate modern laser-based ultrasound techniques for ex-situ measurement of residual stress (a common deleterious feature in advanced manufactured parts).

We successfully advanced a novel in-situ acoustic based melt pool interrogation diagnostic developed by Pennsylvania State University. A system was implemented at Lawrence Livermore National Laboratory Advanced Manufacturing Laboratory. We created a new in-situ eddy current based subsurface temperature monitoring diagnostic and demonstrated it in a laboratory setting in collaboration with Michigan State University. And we demonstrated a novel ex-situ laser-based ultrasound technique for characterizing applied and residual stress working with University of Colorado, Boulder.

Mission Impact

This LDRD project resulted in numerous positive impacts on the Laboratory missions. First, the new technologies developed around in-situ measurements during advanced manufacturing, specifically metal laser-powered-bed-fusion, allow significant decrease in time and cost to qualify new parts, print parameters and materials. These advances are critical to realize advanced manufacturing within the Department of Energy and Department of Defense. Second, this project contributed to a strong and active pipeline of high-quality scientists to National Laboratories and the United States Energy/Defense complex which is critical for the Nation's success.

Publications

Morales, Rosa. 2024. "Acoustoelastic characterization of plates using zero group velocity Lamb modes." Abstract. *Applied Physics Letters* 124, no. 8. <https://doi.org/10.1063/5.0183620>. LLNL-JRNL-856256.

Mutswatiwa, Lovejoy. 2024. "High-speed synchrotron X-ray imaging of melt pool dynamics during ultrasonic melt processing of Al6061." *Nature Communications: Materials* 5, no. 143. LLNL-JRNL-872980.

Rosenberg, Ethan. 2025. "Multifrequency Eddy-Current Detection of Fast Transient Thermal Signatures for In-Situ Monitoring Applications", *Journal of Applied Physics*, LLNL-JRNL-2009473-DRAFT *J. Appl. Phys.* 138, 154501 (2025) <https://doi.org/10.1063/5.0296071>

Posters

Hernandez, Stephanie. 2025. "Thickness-Independent Ultrasonic Evaluation of Internal Residual Stresses in Additively Manufactured Parts." (Poster Presentation at LLNL Summer Students, LLNL, August). LLNL-POST-2009561.

Abstracts

Rosenberg, Ethan. 2025. "Eddy-Current Detection of Fast Transient Thermal Signatures for Additive Manufacturing Applications." Abstract. *ASNT*, LLNL-ABS-872044.

Presentations

Ethan Rosenberg, 2024, "In-situ Temperature Monitoring Using an Eddy Current Sensor Array with Full Field Capture Method LLNL-PRES-866234." (Presented at ASNT Research Symposium, Pittsburgh, June 2024).

Rosa Morales, 2024, "Laser-Induced Zero Group Velocity Lamb Modes to Characterize Anisotropy in Metals." (Presented at ASNT Research Symposium, Pittsburgh, June 2024).

Rosa Morales, 2024, "Thermo-acoustoelastic Characterization of Plates using Zero Group Velocity Lamb Waves LLNL-PRES-864012." (Presented at ASA, Ottawa, May 2024).

Niket Pathak, 2024, "Thermo-acoustoelastic Characterization of Plates using Zero Group Velocity Lamb Waves LLNL-PRES-865923." (Presented at ASNT Research Symposium, Pittsburgh, June 2024).

Ethan Rosenberg, 2025, "Eddy-Current Detection of Fast Transient Thermal Signatures for Additive Manufacturing Applications." (Presented at ASNT Research Symposium, Indianapolis, IN, June 2025).

Niket Pathak, 2025, "Effects of Temperature and Stress on Zero Group Velocity Lamb Modes and their Role in Material Characterization." (Presented at ASNT Research Symposium, Indianapolis, IN, June 2025).

Nathan Kizer, 2025, "High-throughput In-Situ Ultrasonic Monitoring of Melt Pool Dynamics and Phase Transformations in Laser Additive Manufacturing." (Presented at ASNT Research Symposium, Indianapolis, IN, June 2025).

Lei Peng, 2025, "In-Situ Dynamic Temperature Monitoring For Additive Manufacturing With Eddy Current Nondestructive Testing." (Presented at ASNT Research Symposium, Indianapolis, IN, June 2025).

Rosa Morales, 2025, "Laser-Induced Zero Group Velocity Lamb Modes to Characterize Residual Stress In Additively Manufactured Titanium Plates." (Presented at ASNT Research Symposium, Indianapolis, IN, June 2025).

23-ERD-010: Forecasting and Mitigating the Impacts of Climate Change on Renewable Energy Resources and Grid Reliability

Project Overview

Renewable energy generation, particularly from wind turbines and solar photovoltaic (PV) panels, represents a growing portion of U.S. and global generation capacity. Capacity expansion planning models, which are used to plan for investments in energy generation and transmission infrastructure on a multi-decade time horizon, are crucial to ensure resource adequacy with increased wind and solar PV deployment. In this project, we combined high-resolution climate projections with LLNL's stochastic capacity expansion planning model to improve energy infrastructure planning under future uncertainty, with a focus on reliable renewables deployment. We achieved three objectives, including (1) updating LLNL's Climate-to-Infrastructure Computational Pipeline, (2) assessing potential weather impacts on renewable energy resources in the western U.S., and (3) performing novel capacity expansion planning studies for renewable resource droughts and offshore wind deployment in California.

Mission Impact

This project addresses DOE's energy and environmental security mission by helping to plan for critical energy infrastructure that is resilient to natural hazards. Moreover, it contributes to the LLNL mission of Energy Security in two important ways. First, we have demonstrated a novel capability for stakeholders to plan for reliable renewable energy investments under future uncertainty. We have also used this capability to explore scientific questions at the intersection of climate and energy infrastructure planning. We built upon LLNL's Core Competency in Earth and Atmospheric Science by increasing collaboration between experts in renewable energy, climate science, and energy infrastructure. This project led to "Incubator" funding from the DOE Wind Energy Technologies Office (WETO) and is of particular interest to the DOE Office of Electricity (OE) going forward. We have also worked with the LLNL Office of External and Government Affairs (OGEA) to explore potential future work with relevant California government agencies such as the California Energy Commission (CEC).

Publications

Lee, Hsiang-He, Robert Arthur, Jessica Wert, Jean-Christophe Golaz, Jishi Zhang, Matthew Signorotti, and Jean-Paul Watson. 2025. "Accounting for Renewable Resource Droughts in Energy Infrastructure Planning for California, Part I: Present and Future Drought Assessment." In the Proceedings of IEEE Innovations in Smart Grid Technologies - Latin America, Panama City, Panama, September. LLNL-CONF-2007497.

Wert, Jessica, Hsiang-He Lee, Robert Arthur, Matthew Signorotti, Jean-Paul Watson, and Jean-Christophe Golaz. 2025. "Accounting for Renewable Resource Droughts in Energy Infrastructure Planning for California, Part II: Nodal Capacity Expansion Planning." In the Proceedings of IEEE Innovations in Smart Grid Technologies - Latin America, Panama City, Panama, September. LLNL-CONF-2007765.

Lee, Hsiang-He, Robert Arthur, Jean-Christophe Golaz, Jessica Wert, Matthew Signorotti, and Jean-Paul Watson. 2025. "Assessment of Climate Change Impacts on Renewable Energy Resources in Western North America." *Energies* 18, no. 13 (July): 3467. <https://doi.org/10.3390/en18133467>. LLNL-JRNL-860334.

Arthur, Robert, Jean-Christophe Golaz, Hsiang-He Lee, Jessica Wert, Matthew Signorotti, and Jean-Paul Watson. 2025. "High-resolution climate model datasets for energy infrastructure planning in a renewable-dependent future." *Journal of Renewable and Sustainable Energy* 17, (May): 032301. <https://doi.org/10.1063/5.0254086>. LLNL-JRNL-2000972.

Posters

Signorotti, Matthew. 2024. "Computational Pipeline Predicts Solar and Wind Energy Availability under Various Climate Change Projections." (Poster Presentation at Battelle Innovations in Climate Resilience Conference, Washington, DC, April). LLNL-POST-866482.

Zhang, Jishi, Hsiang-He Lee, Jean-Christophe Golaz, Robert Arthur, Matthew Signorotti, Peter Bogenschutz, Minda Monteagudo, Paul Ullrich, Jessica Wert, Stephen Po-Chedley, Philip Cameron-smith, and Jean-Paul Watson. 2025. "Evaluating E3SM for Energy Applications." (Poster Presentation at E3SM All-Hands Meeting, Bethesda, MD, August). LLNL-POST-2010606.

Presentations

Robert Arthur, Jean-Christophe Golaz, Hsiang-He Lee, Jessica Wert, Thomas Edmunds, Matthew Signorotti, Jean-Paul Watson, 2024, "Approaches to Forward Looking Datasets: The Energy Exascale Earth System Model (E3SM)." (Presented at Energy Systems Integration Group Forecasting & Markets Workshop, Salt Lake City, UT, June 2024).

Hsiang-He Lee, Robert Arthur, Jean-Christophe Golaz, Thomas Edmunds, Jessica Wert, Matthew Signorotti, Jean-Paul Watson, 2024, "Assessment of climate change impacts on renewable energy resources in the Western Interconnection Region." (Presented at American Meteorological Society Annual Meeting, Baltimore, MD, January 2024).

Jean-Christophe Golaz, Robert Arthur, Matthew Signorotti, Thomas Edmunds, Hsiang-He Lee, Jean-Paul Watson, 2024, "Evaluating DOE's Energy Exascale Earth System Model (E3SM) for renewable wind and solar energy production." (Presented at American Meteorological Society Annual Meeting, Baltimore, MD, January 2024).

Robert Arthur, 2024, "Forecasting and mitigating the impacts of climate change on renewable energy resources and grid reliability." (Presented at LLNL Physical & Life Sciences External Review Committee Meeting, Livermore, CA, June 2024).

Robert Arthur, Jean-Christophe Golaz, Hsiang-He Lee, Jessica Wert, Thomas Edmunds, Matthew Signorotti, Jean-Paul Watson, 2024, "High-Resolution Climate Datasets for Renewable Resource Assessment and Capacity Expansion." (Presented at Bridging the Gap Between Atmospheric Science and Grid Integration Workshop, Arvada, CO, March 2024).

Jessica Wert, Robert Arthur, Jean-Paul Watson, 2024, "Offshore wind in climate-informed capacity expansion planning." (Presented at Battelle Innovations in Climate Resilience Conference, Washington, DC, April 2024).

Matthew Signorotti, 2024, "Computational Pipeline Predicts Solar and Wind Energy Availability under Various Climate Change Projections." (Presented at INFORMS Annual Meeting, Seattle, WA, October 2024).

Robert Arthur, 2023, "Forecasting and Mitigating the Impacts of Climate Change on Renewable Energy Resources and Grid Reliability." (Presented at LLNL Global Security External Review Committee Meeting, Livermore, CA, May 2023).

Hsiang-He Lee, Robert Arthur, Jean-Christophe Golaz, Matthew Signorotti, Jessica Wert, Jean-Paul Watson, 2025, "Using Multiple High-Resolution Datasets to Benchmark the Energy Exascale Earth System Model (E3SM) for Renewable Resource Assessment." (Presented at American Meteorological Society Annual Meeting, New Orleans, LA, January 2025).

Code

Signorotti, Matthew. 2025. *Renewables Availability Pipeline v. 0.1*.

23-ERD-011: Robust Four-Dimensional Imaging Through Structured Illumination Plenoptics

Project Overview

This research was motivated by a need in the high temperature material testing community for an *in-situ* 3D imaging capability that could measure material topography at very high temperatures (2000C+) where object incandescence interferes with available techniques. The captured data would provide information about material recession and/or failure in experiments like laser ablation and in hypersonic wind tunnel testing. To address this need, a combination of structure light illumination and plenoptic (SLIP) imaging was proposed. In this imaging scheme, an optical pattern is projected using a pulsed laser as the illumination source. That pattern is then measured with a plenoptic camera. The imaged distortion of that pattern can be interpreted to reveal the 3D topography of the underlying sample. The camera can be time gated and spectrally filtered to reject most object incandescence to operate well at high temperatures.

Toward this goal, we developed SLIP imaging. This includes building a pulsed structured light illuminator, a plenoptic camera, software to analytically interpret the results, and a trained machine learning algorithm to interpret results based on empirical training data. The resulting system was demonstrated in a laboratory setting (TRL4) with spatial resolution better than z/z_0 of 0.2%, where z is the depth resolution and z_0 is the standoff distance (2mm resolution from 1m away). The system was then deployed in the LLNL EMIT wind tunnel facility for testing at high temperature (TRL6). Those tests were successful, demonstrating 3D imaging of ceramic material recession at temperatures exceeding 2000C.

Mission Impact

The new SLIP imaging capability allows for real-time measurement of 3D shapes at extreme conditions. The technology has been transitioned into the LLNL EMIT hypersonic wind tunnel diagnostic portfolio, which is also deployable to support DoD field testing. This has direct impact for LLNL Mission Delivery in Multi-Domain Deterrence, where the SLIP data provides previously unobtainable material topography data for hypersonic material response and flight modeling. It also informs material and manufacturing S&T with critical test data to understand why/how/when materials survive or fail in extreme environments. This has impacts spanning modeling, S&T, R&D, and manufacturing development across the whole TRL range.

Publications

Davenport, Dominique, Scott Steinmetz, Benjamin Goldberg, and Erik Busby. 2025. "Advancing 3D surface imaging: single-axis structured light illumination plenoptic camera with machine learning integration." *Optics Express* 33, no. 12 (June): 25233-25247. <https://doi.org/10.1364/oe.558901>. LLNL-JRNL-2004824.

Posters

Davenport, Dominique, Scott Steinmetz, Ben Goldberg, and Erik Busby. 2024. "Structured Light Plenoptic Camera for Dynamic Surface Topography." (Poster Presentation at PLS Postdoc Poster Symposium, Livermore, CA, August). LLNL-POST-867903.

Abstracts

Goldberg, Benjamin, Erik Busby, Rich Shuttlesworth, Jordan Lum, Lionel Keene, Spencer Jeppson, Fred Ellsworth, Kambiz Salari, and Aric Rousso. 2024. "Optical Diagnostics Available in the Lawrence Livermore National Laboratory Energy Matter Interaction Tunnel (EMIT)." Abstract. *Laser Applications to Chemical, Security and Environmental Analysis*, LLNL-CONF-861875.

Presentations

Scott Steinmetz, Madeline Smotzer, Spencer Jeppson, Erik Busby, Kambiz Salari, G. Fred Ellsworth, Rich Shuttlesworth, Aric Rousso, Ben Goldberg, 2024, "High Temperature Material Characterization in a Shearing Environment at the LLNL Energy Matter Interaction Tunnel (EMIT)." (Presented at Hypersonic Technology & Systems Conference, North Logan, UT, September 2024).

Dominique Davenport, Scott Steinmetz, Ben Goldberg, Erik Busby, 2024, "Structured Light Plenoptic Camera for Dynamic Surface Topography Measurement." (Presented at University Consortium for Applied Hypersonics Forum, Alexandria, VA, August 2024).

Erik Busby, 2024, "Optics at the Intersection of Chemistry, Materials, and Physics." (Presented at Invited Chemistry Departmental Seminar, University of California, Davis, October 2024).

23-ERD-012: Climate-Driven Changes to Host Nutrition May Impact the Emergence and Phenotype of Viral Variants

Project Overview

Undernutrition and micronutrient deficiencies, particularly selenium deficiency (Se def), have been recognized as critical factors that compromise host immune responses and increase susceptibility to viral infections. Deficits in host nutrition can increase the virulence and evolution rate of viruses. The aim of this study was to assess the impact of Se def on viral emergence and evolution using two recently emergent viruses, severe acute respiratory syndrome coronavirus 2 (SARS CoV-2) and Zika virus (ZIKV) using established mouse models that recapitulate human disease. In-depth genetic analysis was used to define the dynamics of viral variant emergence in Se def mice compared to the genetic diversity in mice fed a Se adequate diet. For each diet group the strength of the host immune response was analyzed, and virus was quantitated in infected tissues. Virus derived from repeated passage of SARS CoV-2 in Se def mice had significantly higher genetic diversity throughout the genome including multiple mutations known to impact viral virulence and that were subsequently detected in Omicron lineages. Se def passaged SARS CoV-2 was generally more pathogenic in aged mice and had increased impact on the immune response. Results for ZIKV differed in that no significant difference in overall viral genetic diversity was detected according to diet group, however, unique mutations were detected in a subset of mice fed a nutrient deficient diet, higher titers of ZIKV were found in the brains of mice fed a diet deficient in both Se and vitamin E, and higher mortality was observed for this diet group. Immune analysis detected widespread changes for nutrient deficient mice infected with ZIKV. In summary, data from this project support the hypothesis that the passage of viruses through host populations that are selenium deficient and/or severely malnourished can alter viral evolution and virulence.

Mission Impact

Data from these comprehensive experiments provide important information about the potential for increased emergence of viral mutations that might be anticipated to occur more frequently with global climate disruption. Increased understanding of viral genetic diversity generated by host malnutrition and mineral deficiency provides guidance for the design of effective therapeutics and countermeasures. Predicting how viruses might evolve in hosts living under chronic environmental stress conditions improves the security and resilience of the nation and its critical infrastructure against biological agents.

Publications

Oluwasemowo, Olukunle O., Monica E. Graham, Deepa K. Muruges, and Monica K. Borucki. "Improved Zika Virus Plaque Assay Using Vero/Tmprss2 Cell Line." *Microbiology Spectrum* 13, no. 1 (2025): e01624-24.

Presentations

Borucki, Monica. 2024, "Recovering Viral Population Diversity to Improve Biosurveillance and Predict Viral Emergence." (Presented at Workshop on Forecasting Zoonotic Emergence Events, LANL, January 2024). LLNL-PRES-859483

Oluwasemowo, Olukunle, Monica Graham, Deepa Muruges, Ashlee Philips, Aram Avila-Herrera, Jeff Kimbrel, Adam Zemla, Dina Weilhammer, Nicole Collette and Monica Borucki. "Climate-Driven Nutritional Changes and Their Impact on the Emergence of Zika Virus Variants", (Presented at African Virology Network Conference 2024, Abuja, Nigeria November 2024). LLNL-PRES-871183

Graham, Monica. 2025, "Impacts of Climate-driven Host Selenium Status on SARS-CoV-2 Pathogenesis and Variant Emergence" (Presented at American Society for Virology Meeting, July 2025); LLNL-CFPRES-2008199

Posters

Oluwasemowo, Olukunle, Monica Graham, Deepa Muruges, Ashlee Phillips, Aram Avila-Herrera, Jeff Kimbrel, Adam Zemla, Nicole Collette, Dina Weilhammer, and Monica Borucki. 2024. "Climate-driven Changes to Host Nutrition May Impact the Emergence and Phenotype of Viral Variants." (Poster Presentation at LLNL PLS Postdoc Poster Symposium, Livermore, CA, August). LLN-POST-868197.

Graham, Monica, Olukunle Graham, Deepa Muruges, Nicole Collette, Dina Weilhammer, and Monica Borucki. 2024. "Climate-driven Changes to Host Selenium Status May Impact SARS-CoV-2 Pathogenesis and Variant Emergence." (Poster Presentation at LLNL PLS Postdoc Poster Symposium, Livermore, CA, August). LLNL-POST-868208

Oluwasemowo, Olukunle, Monica Graham, Deepa Muruges, Ashlee Phillips, Aram Avila-Herrera, Jeff Kimbrel, Adam Zemla, Dina Weilhammer, Nicole Collette and Monica Borucki. 2025. Climate-Driven Nutritional Changes and Their Impact on the Emergence of Zika Virus Variants. Presented at American Society for Virology Conference, Montréal, Québec, Canada, July, 2025. LLNL-POST-2008004

Olukunle Oluwasemowo, Monica Graham, Deepa Muruges, Ashlee Phillips, Aram Avila-Herrera, Jeff Kimbrel, Adam Zemla, Dina Weilhammer, Nicole Collette and Monica Borucki. 2025. "Weather Pattern - Induced Changes to Host Nutrition May Impact the Emergence and Phenotype of Zika Virus Variants" (Presented at PLS Annual Postdoc Poster Presentation, June 24, 2025). LLNL-POST-2007769

23-ERD-013: Host-Directed, Bioelectronic Immunomodulation for Protection Against Emerging Pathogens

Project Overview

Acute care of patients with severe infections often relies on systemic administration of pharmaceuticals and monitoring of complex physiological symptoms to identify immune system dysfunction, which can lead to increased mortality. Furthermore, determining disease-specific treatment plans often leads to a delay in patient care. To address this, we proposed an immune modulation system that electrically detects and responds to a patient's immune system status, creating an agnostic means of treating illness and infection. Two pieces of hardware were developed for this task: a minimally-invasive sensor and a vagus nerve stimulator. Stimulation of the vagus nerve is known to modulate the immune system. The sensor is a microfabricated, silicon-based microneedle array capable of interfacing with interstitial fluid to detect small molecules such as inflammatory proteins (cytokines) and pharmaceuticals (vancomycin). Process optimization to manufacture the needles refined the silicon etch process, creating needle patches long enough to penetrate skin and reach interstitial fluid. The needles were tested for mechanical strength and stability, and did not shatter when inserted into skin models. The needles are coated with a thin film metal, turning them into electrodes for electrochemical sensing of our target molecules. We hybridized aptamers to the surface of the electrode to act as the sensing layer and were able to detect changes in the conformation of the aptamer electrochemically in the presence of the target molecule. The stimulator was a cuff electrode that encircled the vagus nerve. Rodent studies were conducted in which rodents were exposed to an inflammatory event and vagus nerve stimulation (VNS) was applied. It was demonstrated that optimized electrical stimulation of the vagus nerve created measurably different levels of cytokines in blood samples, and certain cytokines released during the inflammatory event were either upregulated or downregulated. In sum, this project successfully developed new platforms and technologies that can, with further development, enable better temporal insight into biomarker changes in the body, letting healthcare providers know of possible immune system dysfunction before they are detected physiologically. We also demonstrated the value of VNS and its possible use in treating immune system response to inflammation and illness.

Mission Impact

With the increasing risk of biothreats globally, innovative solutions are required to support quick response and bioresiliency. This research is directly related to developing technology and tools to meet such future national security challenges, and enables agnostic response to biothreats by diagnosing and treating people regardless of the specific type of biothreat. This research generated a new sensing platform (wearable microneedles), the development of which is currently in discussions to support federal agencies such as Department of Defense. Such minimally invasive, wearable technologies are of interest in supporting the warfighter, whether by identifying the presence of infection or biothreats or by tracking human performance. There is also possible tie-ins to agencies such as NASA, as wearable technologies capable of examining small changes within the body are of interest when considering spaceflight. The microneedle platform is an enabling technology with a wide possible range of applications in support of LLNL missions and, more generally, these other federal agencies. The microneedles can be modified to detect other biomarkers of interest and can be used in similarly broad applications.

Publications

Zhou, Jenny, Erik Mukerjee, Kathy Jackson, Sarah Sahota, Jose Hernandez, Anna Ivanovskaya, Georgia Lawlor, Vassilis Koliatsos, and Allison Yorita. 2025. "Fabrication Challenges and Process Improvements for 650 Micrometer-Long Silicon Microneedles for Biosensing in Interstitial Fluid." In the Proceedings of IEEE Biosensors 2025, San Diego, CA, August. LLNL-CONF-2003867.

Posters

Baker, Megan, Anna Ivanovskaya, Allison Yorita, and Samantha Santacruz. 2024. "Carbon nanotube surfaces functionalized with aptamers for use in real time quantification of cytokines in the brain." (Poster Presentation at Neuroelectronic Interfaces Conference (GRC), Galveston, TX). LLNL-POST-861158.

Baker, Megan, Sarah Sahota, Anna Ivanovskaya, Allison Yorita, and Samantha Santacruz. 2024. "Electrochemical sensing of cytokines utilizing carbon nanotube fiber-based electrodes." (Poster Presentation at Material Research Society 2024 Spring Meeting & Exhibit, Seattle, WA). LLNL-POST-863085.

Zhou, Jenny, Erik Mukerjee, Kathy Jackson, Sarah Sahota-Dhillon, Jose Hernandez, Anna Ivanovskaya, Georgia Lawlor, Vassilis Koliatsos, and Allison Yorita. 2025. "Fabrication Challenges and Process Improvements for 650 Micrometer-Long Silicon Microneedles for Biosensing in Interstitial Fluid." (Poster Presentation at IEEE Biosensors 2025, San Diego, CA, August). LLNL-POST-2009174.

Zhou, Jenny, Sarah Sahota, Anna Ivanovskaya, Jose Hernandez, Georgia Lawlor, Sadid Khan, Vassilis Koliatsos, and Allison Yorita. 2024. "Host-directed, bioelectronic immunomodulation for protection against emerging pathogens." (Poster Presentation at DTRA CBD S&T Conference, Fort Lauderdale, FL, December). LLNL-POST-871143.

Zhou, Jenny, Anna Ivanovskaya, Sarah Sahota-Dhillon, Jose Hernandez, Georgia Lawlor, Sadid Khan, Vassilis Koliatsos, and Allison Yorita. 2025. "Towards closed-loop bioelectronic immunomodulation for agnostic protection against emerging pathogens." (Poster Presentation at Military Health System Research Symposium, Kissimmee, FL, August). LLNL-POST-2009461.

23-ERD-014: Precision Polishing of Spheres Via In-Situ Process Monitoring and Machine-Learning-Based Optimization

Project Overview

Precision polishing for high surface finish is a vital step in the making of many high-tech components for optical and semiconductor modules as well as for wide ranging experimental samples for HED science that is at the core of LLNL's mission. In particular, the fabrication of extremely smooth and round spheres comprised of low atomic number materials (low-Z such as high-density carbon or HDC, beryllium, hydrocarbon polymers, etc.) for Inertial Confinement Fusion (ICF) is entirely reliant on specialized polishing processes to achieve the surface smoothness.

This project primarily sought to implement a multi-sensor fusion approach for real-time monitoring of the precision V-groove polishing process that is used for achieving the near-perfect surface finish of ablator spheres with a goal of extracting correlation between the relevant signals in the sensor data and key aspects of the process. Additionally, new diamond polishing plate microstructures were explored with the goal of developing a more efficient polishing process which creates significant value for the program. Confocal and interferometric optical surface characterization was used extensively to obtain the final performance metrics and analysis of signals from 3 sensors - time-synced vibration, acoustic and optical imaging sensors - was done using machine learning (ML) based algorithms.

The HDC capsule is indeed the most impactful component of an ICF ignition target, and the surface quality of the capsule is paramount. The requirements are extremely stringent (surface roughness of a few nm, no pits $>1\mu\text{m}^3$) which required the finishing process, comprised of the steps of lapping and polishing, to operate flawlessly and efficiently. In that regard this LDRD project provided the following significant advances:

1. ~3x faster lapping process while retaining the same high quality, which has already been inducted into the production of HDC capsules for ICF ignition targets.
2. Successful development of fine lapping process as a viable and ~3x faster alternative to the polishing step while retaining the same high quality understanding of the kinetics of achieving the generic surface smoothness (as quantified by the rms value of surface asperities).
3. Mechanism of formation of small pits which is key for sustaining high quality.

Mission Impact

Ultra-precision surface finishing is a central requirement for a number of HED and ICF related projects where unprecedented surface finishes are required for a very large range of scales – meter-scale optics to millimeter sized spheres and micron-thick films for targets. It is crucial to nurture and expand the state-of-the-art knowledge that exists at LLNL in the field with infusion of emerging fields of sensing and using more sophisticated large-data processing. This project focuses on the science that “helps position the Laboratory to support emerging needs and provides opportunities for program growth.” Our project is also within the Core Competency (HED and ICF Programs) as it

sustains excellence in critical areas that distinguish the Laboratory and enables us to meet enduring mission needs.

These findings and the new methodologies developed here would have impact on other fields (optical and semiconductor) with stringent surface requirements as well.

Publications, Presentations, Patents

Galla, S. et al, 2024. "Detecting anomalous motions in ultraprecision shell-polishing process combining unsupervised spectral-band identification and Explainable-AI." *J. Manuf. Sys*, 75, 278-287-2024

Tiwari, A. et al, 2025. "Precision Polishing of Ablator Capsules via in situ Process Monitoring and Machine Learning–Based Optimization. *Fus. Sci. Tech.*, 81, 219-231, 2025.

Alexos, A. et al, Nuclear Fusion Diamond Polishing Dataset, Conference paper, Nuerips, 2024.

Canacao, S. et al, "Efficient screening of rare large pit anomalies on polished surfaces using a minimalist sampling scheme." 2025. *J. Manuf. Proc.*, 147, 80-87.

Galla, S. et al, "Domain-Adaptive ML for Surface Roughness Predictions in Nuclear Fusion." Conference paper, Nuerips, 2024

Alexos, A. et al, 2023. "Machine Learning–Enhanced Prediction of Surface Smoothness for Inertial Confinement Fusion Target Polishing Using Limited Data." Conference paper, Nuerips, 2023.

Jin, S. et al, "Vibration Signal-Assisted Endpoint Detection for Long-Stretch, Ultraprecision Polishing Processes." 2023. *J. Manuf. Sci. Eng.*, 145(6), 061007.

Galla, S. et al , Scalable Anomaly Detection in Batch Polishing Processes for Inertial Confinement Fusion Shells, Conference paper, ICML Workshop for AI4Science, 2024.

Bhandarkar, S., Accelerometer-based monitoring of HDC capsule polishing, 25th Target Fabrication Specialists Meeting, San Diego, CA. August 25th – 29th, 2024.

Bukapatnuam, S., Accelerometer-based monitoring of HDC capsule polishing, International Academy of Manufacturing Engineering (72nd CIRP General Assembly) Aug 2023.

Galla, S., Machine Learning-Enhanced Prediction of Surface Smoothness for Inertial Confinement Fusion Target Polishing Using Limited Data, World Congress on Artificial Intelligence in Materials and Manufacturing, AIM, June 2024.

Bhardwaj, K, Scalable Anomaly Detection in Batch Polishing Processes for Inertial Confinement Fusion Shells, ICML 2024-AI4Science, Vienna Jul, 2024.

Tiwari, A., Precision Polishing of Ablator Capsules via in situ Process Monitoring and Machine Learning–Based Optimization, 2023 Texas A&M Conference on Energy, September 2023.

23-ERD-015: Establishing a Design Hub for Tokamak Fusion Reactor Divertor Systems

Project Overview

Recognizing the urgent need for new energy sources and energy security, nations and industry are moving rapidly to design and build fusion power plants. The approach to fusion closest to delivering power to the grid is widely considered to be the magnetic tokamak. Inside a tokamak power plant, the walls will experience extreme heat loads; the potential for melting of the walls poses a critical risk to the fusion energy mission. The part of the wall that must handle the highest heat loads is called the divertor, which if damaged could cost hundreds of millions of dollars to repair. The current divertor designs are vulnerable under such conditions. Improved divertor configurations, optimized under considerable uncertainties and constraints, are needed as a critical part of an integrated reactor design. Lawrence Livermore National Laboratory (LLNL) is a world leader in tokamak divertor science but needs to adapt that science into practical and efficient tools to accelerate optimal new divertor design and safe operation.

This project demonstrated automated inference of divertor plasma model parameters with uncertainties from the National DIII-D tokamak experimental data using Bayesian Optimization. Results have been presented at multiple conferences and in a submitted publication. Modifications were made to the LLNL code UEDGE to create a new workflow that incorporates bolometry measurements in the model. Application of this new workflow to experiments highlighted a potential issue with matching radiation between code and experiment and provides a new tool to analyze this discrepancy. Global optimization search methods were implemented to infer model parameters, accelerated using parallel computation techniques. We developed new synthetic diagnostics for experimental validation, and automated workflows by developing tools to gather experimental data, optimize computational meshes, sped up and automatically converge complex simulations and manage the resulting datasets. These advances are integrated into the UETOOLS toolbox to enhance the productivity of future applications of UEDGE to tokamak experiments and divertor design.

Mission Impact

This project fits within the Energy Security mission. This research advances the mission of DOE Fusion Energy Sciences to build the scientific and technological foundations necessary for developing a fusion energy source: Our new capability to automatically infer model parameters from experimental data enhances analysis of current experiments and provides the basis for digital twins of future fusion power plants. The inference techniques and tools developed are adaptable to meet future national security challenges.

Publications

Dudson, Ben, Mike Kryjak, Hasan Muhammed, Peter Hill, John Omotani. 2024. "Hermes-3: Multi-component plasma simulations with BOUT++" *Comp. Phys. Comm.* 296 108991
<https://doi.org/10.1016/j.cpc.2023.108991>

Fu, Yichen, Ben Dudson, Xiao Chen, Maxim Umansky, Filippo Scotti, Tom Rognlien, Anthony Leonard. 2025. “Statistical inference of anomalous thermal transport with uncertainty quantification for interpretive 2-D SOL models” Y Fu *et al* 2026 *Plasma Phys. Control. Fusion* 68 015010DOI 10.1088/1361-6587/ae2b0b

Oral Presentations

Dudson, B. D., M. V. Umansky, T. Rognlien, F. Scotti, X. Chen, R. Li, C. Santiago, D. Osei-Kuffuor. 2022. “B. D. Dudson, M. V. Umansky, T. Rognlien, F. Scotti, X. Chen, R. Li, C. Santiago, D. Osei-Kuffuor”. Presentation to the National DIII-D Divertor Science and Innovation (DSI) meeting, December 6th.

Umansky, M. V., B. I. Cohen, I. Joseph. 2023. “Tokamak boundary plasma turbulence and its implications for plasma-material interactions” Presentation to the International ITPA DivSOL meeting, Knoxville, TN, 6-9 June. LLNL-PRES-849931

Poster Presentations

Dudson, B. D., M. Kryjak, H. Muhammed, P. Hill, J. T. Omotani. 2023. “Multi-component transport and turbulence simulations with Hermes-3” Poster, Transport Task Force workshop, Madison, WI. May 2-5. LLNL-POST-847824

Umansky, M. V., B. D. Dudson, T. D. Rognlien, F. Scotti. 2023. “Interpretive modeling of heat transport in the boundary of DIII-D”. Poster, Transport Task Force workshop, Madison, WI. May 2-5. LLNL-POST-854898

Dudson, B. D., M. V. Umansky, T. Rognlien, F. Scotti, X. Chen, R. Li, A. Friedman. 2022. “Developing tools to accelerate divertor design and full-power operation” Poster, APS-DPP conference in Spokane, OR. October 17-21. LLNL-POST-840297

Dudson, B. D., M. V. Umansky, T. Rognlien, F. Scotti, X. Chen, R. Li, A. Friedman. 2022. “Developing tools to accelerate divertor design and full-power operation” Poster, IAEA Technical Meeting, Vienna, Austria. November 7-11. LLNL-POST-840297

Fu, Yichen. 2024. “Statistical inference of anomalous thermal transport with uncertainty quantification in the plasma boundary”. Transport Task Force workshop (April 9-12, <https://conferences.union.wisc.edu/ttf/>) LLNL-POST-862517

Fu, Yichen. 2024. The 5th International Conference on Data-Driven Plasma Science (ICDDPS-5) <https://na.eventscloud.com/website/63026/home/>

Fu, Yichen, Benjamin Dudson, Xiao Chen, Maxim Umansky, Filippo Scotti. 2024. “Statistical inference of anomalous thermal transport with uncertainty quantification in the plasma boundary” APS-DPP.

Chen, Xiao. 2024. "Bayesian Optimization with UQ for Inferring Anomalous Thermal Transport in Fusion Plasma Using UEDGE and DIII-D Data", SIAM NCC Conference
<https://sites.google.com/view/siam-ncc/siam-ncc-conference-2024/posters>

Software

Highly-efficient OpenMP parallelization of costly UEDGE Jacobian matrix (CP02690)

New capabilities added to UETOOLS analysis suite (<https://github.com/LLNL/UETOOLS>) enabling (a) Bayesian inference of model parameters from data; (b) forward modeling of Bolometer diagnostic from UEDGE simulations. CP02706

23-ERD-016: Systems-To-Atoms Enabling Hydrogen for Climate Security

Project Overview

The transition to clean energy requires reliable ways to store, move, and use hydrogen, which can help reduce emissions from heavy-duty transportation and other hard-to-decarbonize sectors. However, existing hydrogen storage and delivery methods each face challenges: compressed hydrogen requires expensive pipelines, liquid hydrogen suffers from energy losses, and liquid carriers require efficient catalysts to release hydrogen. To address these issues, our team created a new “systems-to-atoms” framework that links large-scale energy system models with detailed material studies. This approach allowed us to evaluate how real-world factors such as demand fluctuations, regional differences, and operating conditions affect hydrogen delivery options.

Using this framework, we compared different methods for transporting hydrogen in California, including compressed gas, cryogenic liquid, and liquid organic hydrogen carriers. The results showed that no single option is always best; instead, the most effective solution depends on the intended use and location. By connecting material performance to system needs, our research identified key parameters that determine cost, efficiency, and durability. These findings demonstrate the importance of designing hydrogen technologies with both system-level and material-level considerations in mind, enabling more reliable and cost-effective deployment of clean energy infrastructure.

Mission Impact

This work directly supports LLNL’s mission in Energy Security by providing a new modeling and simulation capability that bridges materials science and systems analysis. The S2A framework positions LLNL as a leader in multi-scale integration, enabling rapid response to environment-specific infrastructure needs. For DOE and NNSA missions, the project advances critical infrastructure by informing cost-performance trade-offs, guiding material development, and providing validated tools for decision-making to meet future national security challenges. Beyond hydrogen, the framework can be generalized to other mission areas requiring system-material co-design, such as energy resiliency management, advanced manufacturing, and resource security. The project also fostered cross-directorate collaboration and workforce development, integrating expertise from PLS, ENG, COMP, and GS, and establishing new partnerships with academia and industry.

Publications, Presentations, and Patents

Yuan, Mengyao, Giovanna Bucci, Tanusree Chatterjee, Shyam Deo, John R. Kitchin, Carl D. Laird, Wenqin Li et al. "Integrated Systems-to-Atoms (S2A) Framework for Designing Resilient and Efficient Hydrogen Infrastructure Solutions." *Energy & Fuels* 39, no. 14 (2025): 7119-7128.

Deo, Shyam, Wenyu Sun, Tanusree Chatterjee, Thomas Moore, Mengyao Yuan, Matthew J. Mcnenly, Sneha A. Akhade, and Giovanna Bucci. "Cross-scale catalyst modeling applied to H2

storage and release via formic acid." *Industrial & Engineering Chemistry Research* 64, no. 3 (2025): 1439-1448.

Sunshine, Ethan M., Giovanna Bucci, Tanusree Chatterjee, Shyam Deo, Victoria M. Ehlinger, Wenqin Li, Thomas Moore et al. "Multiscale optimization of formic acid dehydrogenation process via linear model decision tree surrogates." *Computers & Chemical Engineering* 194 (2025): 108921.

Sunshine, Ethan M., Carolina Colombo Tedesco, Sneha A. Akhade, Matthew J. McNenly, John R. Kitchin, and Carl D. Laird. "Hyperplane decision trees as piecewise linear surrogate models for chemical process design." *Computers & Chemical Engineering* (2025): 109204.

Akhade, Sneha, and Matthew Mcnenly. 2023. system2atoms (S2A), v. 0.1.
<https://github.com/LLNL/systems2atoms>

23-ERD-017: Scalable Methods for Contact with Optimization

Project Overview

Engineering and physics codes often used in analyses exhibit many instances of unilateral contact mechanics, which fall under the umbrella of nonsmooth systems of nonlinear equations. These codes have relied on parallel direct solvers, which have poor scalability and, hence, limit the resolution and extent of contact analyses as well as the embedding of contact analyses in design processes and artificial intelligence (AI) workflows.

This integrative R&D project was aimed at solving large-scale contact and contact design problems using high-performance computing (HPC) and was structured along three salient research thrusts: (i) nonlinear nonsmooth solvers for contact mechanics, (ii) algebraic multigrid (AMG) linear solvers, and (iii) computational models for contact design optimization problems. The homotopy algorithms developed under the first thrust and the filtering AMG method developed under the second thrust reached out *unprecedented computational scales*, namely, up to hundreds of millions of unknown variables and thousands of computational cores on Dane HPC cluster of Livermore Computing facility. The computer codes containing these algorithms were made publicly available in LLNL's MFEM library and are currently integrated within LLNL production codes performing real-world contact analyses. The third thrust developed novel computational design models involving contact mechanics and used optimization algorithms to provide best candidate designs for a couple of real-world assemblies involving multiple parts in contact with one another.

Mission Impact

The project addressed stringent limitations in contact mechanics analyses by providing the scalable computational and algorithmic infrastructure required for such analyses. As a result, the project improved LLNL's programmatic capabilities to simulate assemblies of bodies in contact, which enhances the fundamental understanding of aging nuclear weapons systems. The novel scalable methods and robust HPC solvers developed by this project reduce the amount of human intervention required in the analysis of large number of ensembles and, hence, pave the road towards automated AI workflows that can potentially enhance the safety, security, and effectiveness of the U.S. nuclear weapons stockpile.

Publications

Tucker Hartland, Cosmin Petra, Noemi Petra, Jingyi Wang. 2025. "A scalable interior-point Gauss-Newton method for PDE-Constrained Optimization with Bound Constraints." Wiley Journal of Numerical Linear Algebra with Applications. 30 November 2025 <https://doi.org/10.1002/nla.70040>

Technical Reports

Wang, Jingyi, Cosmin Petra, and Jean-Luc Peterson. 2024. "Constrained Bayesian optimization with merit function." Lawrence Livermore National Laboratory. LLNL-JRNL-1093787.

Wang, Jingyi, Jerome Solberg, Mike Puso, Eric Chin, and Cosmin Petra. 2024. "Design optimization in unilateral contact using pressure constraints and Bayesian optimization." Lawrence Livermore National Laboratory. LLNL-JRNL-1096720.

Presentations

Tucker Hartland, Cosmin Petra, Jingyi Wang, 2024, "A scalable interior-point Gauss-Newton method for PDE- and bound-constrained optimization." (Presented at Gradient-Based Optimization Workshop, Livermore, CA, February 2024).

Tucker Hartland, Cosmin Petra, Jingyi Wang, 2024, "A scalable interior-point Gauss-Newton method for PDE-constrained optimization with bound constraints." (Presented at SIAM Conference on Applied Linear Algebra, Paris, France, May 2024).

Tucker Hartland, Socratis Petrides, Eric Chin, Jingyi Wang, Mike Puso, Jerome Solberg, Tzanio Kolev, Cosmin Petra, 2024, "An interior-point multigrid-based approach for scalable contact mechanics." (Presented at International Conference on Preconditioning Techniques for Scientific and Industrial Applications, Atlanta, GA, June 2024).

Tucker Hartland, Socratis Petrides, Mike Puso, Tzanio Kolev, Jerome Solberg, Cosmin Petra, Eric Chin, Jingyi Wang, 2024, "An interior-point multigrid-based approach for scalable contact mechanics." (Presented at 16th World Congress on Computational Mechanics, Vancouver, Canada, July 2024).

Jingyi Wang, 2024, "Local convergence of a sequential quadratic programming method for a class of nonsmooth nonconvex objectives." (Presented at 2024 INFORMS Optimization Society Conference, Houston, Tx, March 2024).

Tucker Hartland, 2025, "A scalable interior-point Gauss-Newton method for PDE- and bound-constrained optimization." (Presented at MFEM Community Workshop, Portland, Oregon, September 2025).

Mike Puso, 2025, "AMG with Filtering for Large-Scale Contact Mechanics Interior-Point Optimization." (Presented at International Conference on Computational Contact Mechanics, Munich, Germany, June 2025).

Socratis Petrides, 2025, "AMG with Filtering – An Efficient Preconditioner for Large-Scale Contact Mechanics Interior-Point Optimization." (Presented at USNCCM18, Chicago, IL, July 2025).

Socratis Petrides, 2025, "AMG with Filtering – An Efficient Preconditioner for Large-Scale Contact Mechanics Interior-Point Optimization." (Presented at MFEM Community Workshop, Portland, Oregon, January 2025).

Mike Puso, 2025, "On a structure preserving approach for frictional contact." (Presented at USNCCM18, Chicago, IL, July 2025).

Code

Hartland, Tucker, and Cosmin Petra. 2025. *Continuation and homotopy solvers*.

23-ERD-018: PowderJet: An Agile System for High-Quality Metal-Powder Production

Project Overview

Leading metal 3D printing techniques require specially prepared spherical metal powders to produce high quality functional parts. The performance of 3D-printed metal parts depends on the quality and composition of this input powder, but currently available powder production technologies have technical shortcomings that limit innovation in this field. Within this LDRD project, we developed a new metal alloy powder production platform called PowderJet that produces metal powders in a controlled environment by ejecting liquid metal droplets through a designed nozzle with electromagnetic pulses. This approach is fundamentally different than the uncontrolled way in which other powder-production methods operate. PowderJet complements these other metal powder production methods as it has exquisite powder particle size selectivity, is adaptable to hazardous/reactive metals, and can rapidly produce useful batches of boutique alloy powders that are needed in a research environment. With these advantages, the platform will advance liquid metal jetting and powder metallurgy, as well as enable rapid discovery and optimization of metal powders for metal 3D printing.

Mission Impact

This LDRD project represents a step forward for LLNL's advanced manufacturing capabilities which are integral to mission deliverables and capabilities that meet future national security challenges. Production of metal components often involves specially prepared feedstock materials which can then be transformed into end use components. Increasingly, this is done using advanced manufacturing technologies such as additive manufacturing/3D printing. Within this scope, the project impact can be broken down into two main areas: (1) the project advances metal droplet generator technology useful for metal 3D printing and (2) it advances metal powder feedstock production capabilities, which are necessary for powder-based additive manufacturing technologies. The results of this project will find use in any federal missions that require high quality special powder feedstocks or precise and rapid generation of liquid metal droplets.

Posters

Mooraj, Shahryar. 2024. "Rapid screening of liquid metal wetting for a materials compatibility library." (Poster Presentation at MED Post-doc Poster symposium, LLNL, August). LLNL-POST-868218.

Presentations

Viktor Sukhotskiy, Alexander Baker, Jesse Ahlquist, Shahryar Mooraj, Alexandre Reikher, Eric Elton, Hunter Henderson, 2024, "PowderJet: an agile system for high quality metal powder production." (Presented at Solid Freeform Fabrication Symposium 2024, Austin, TX, August 2024).

Records of Invention

Sukhotskiy, Viktor, Alexander Baker, Jesse Ahlquist, Eric Elton, and Hunter Henderson. 2024. "Method for high performance metal droplet ejection via meniscus control enabled by a versatile multi-part nozzle design." IL-13967.

Sukhotskiy, Viktor. 2024. "Method for selective resolution in metal droplet additive manufacturing via control of multi-orifice nozzle ejections." IL-13885.

Journals

Mooraj et al. 2025. "Rapid screening of liquid metal wetting for a materials compatibility library," *MDPI Metals* Metals 2025, 15(10), 1121; <https://doi.org/10.3390/met15101121>

23-ERD-021: Three-Dimensional Ion Traps to Enable Quantum Error Correctable and Scalable Quantum Computing

Project Overview

Quantum computing has the potential to revolutionize computational capabilities for problems such as chemical reactivity modeling. However, current quantum hardware is limited by the number of quantum bits (qubits) and error rates in the physical quantum operations. This project aimed to overcome some of these limitations by developing a new fabrication platform for ion traps: miniaturized three-dimensional (3D) ion traps using advanced additive manufacturing techniques. The approach leverages two-photon polymerization direct laser writing (2PP-DLW) to fabricate complex 3D trap architectures with sub-micron resolution, enabling stronger ion confinement, higher motional frequencies, and significantly reduced noise compared to conventional 2D planar traps. Over the course of the project, we designed, fabricated, and tested new 3D ion trap structures, developed rapid characterization techniques, and took steps towards establishing a new ion trap testing facility at LLNL. Results demonstrate that the fabrication methodology is compatible with ultrahigh vacuum and cryogenic environments while providing near-state-of-the-art heating rates, thus establishing a novel scalable hardware platform for future ion-based quantum computers.

Mission Impact

This project advanced LLNL's national security mission by leveraging the laboratory's Core Competency in Advanced Materials and Manufacturing to create miniaturized three-dimensional ion traps for quantum computing. Using state-of-the-art additive manufacturing techniques, we demonstrated a new fabrication platform with a pathway to scalable, low-error quantum hardware. Such hardware will enable modeling and simulation capabilities in future quantum coprocessors that address critical challenges in stockpile stewardship science, nuclear threat reduction, and other mission-driven applications for NNSA and DOE. The fabrication methods and infrastructure developed through this work expand LLNL's quantum technology portfolio. The project developed strong research collaborations with leading academic groups in the University of California system, laying the groundwork for future collaborations and workforce development in quantum information science and advanced manufacturing for next-generation national security solutions.

Publications

Xu, Shuqi, Xiaoxing Xia, Qian Yu, Abhinav Parakh, Sumanta Khan, Eli Megidish, Bingran You, Boerge Hemmerling, Andrew Jayich, Kristin Beck, Juergen Biener, and Hartmut Haeffner. 2025. "3D-printed micro ion trap technology for quantum information applications." *Nature* 645 (September): 363-368. <https://doi.org/10.1038/s41586-025-09474-1g>. LLNL-JRNL-2003961.

Posters

Patra, Sayan, Abhinav Parakh, Shuqi Xu, Xiaoxing Xia, Juergen Biener, Hartmut Haeffner, and Kristin Beck. "3D-printed ion traps for scalable quantum information processing." (Poster

Presentation at North American Conference on Trapped Ions, Los Angeles, California, August) 2024). LLNL-POST-867742.

Xu, Shuqi, Xiaoxing Xia, Qian Yu, Abhinav Parakh, Kristin Beck, Boerge Hemmerling, Andrew Jayich, and Hartmut Haeffner. "3D-Printed Micro Ion Trap for Quantum Information Processing." (Poster Presentation at North American Conference on Trapped Ions, Los Angeles, California, August 2024). LLNL-POST-2000496.

Parakh, Abhinav, Shuqi Xu, Xiaoxing Xia, Kristin Beck, Qian Yu, Samanta Khan, Eli Megidish, Bingran You, Juergen Biener, and Hartmut Haeffner. "Additive manufacturing of ion traps for quantum computing." (Poster Presentation at Engineering and Strategic Deterrence Summer Poster Slam, LLNL, Livermore, CA, August 2024). LLNL-POST-848075.

Brzeczek, Merrell, Robert Kwapisz, A. Sawhney, Nisa Kuvvet, C. Zhang, Shuqi Xu, H. Dan, V. Baid, Dongrong Li, Sean Buechele, R.A. Ready, Xiaoxing Xia, Kristin Beck, Juergen Biener, Boerge Hemmerling, Hartmut Haeffner, Dave Patterson, and Andrew Jayich. 2024. "Cryogenic Operation of Micron-scale 3D-printed Ion Traps." (Poster Presentation at North American Conference on Trapped Ions, Los Angeles, California, August). LLNL-POST-2000508.

Brzeczek, Merrell, Sean Buechele, Chaoshen Zhang, Shuqi Xu, Hauxu Dan, Vinay Baid, Dongrong Li, Roy Ready, Xiaoxing Xia, Juergen Biener, Boerge Hemmerling, Hartmut Haeffner, Dave Patterson, and Andrew Jayich. 2023. "Cryogenic System for 3D Printed Ion Traps." (Poster Presentation at European Conference on Trapped Ions, Buckeburg, Germany, September). LLNL-POST-2000507.

Patra, Sayan, Abhinav Parakh, Xiaoxing Xia, Juergen Biener, and Kristin Beck. "3D-printed ion traps for quantum applications." (Poster Presentation at Institutional Postdoctoral Poster Symposium, Livermore, CA, June 2025). LLNL-POST-2007280.

Patra, Sayan, Abhinav Parakh, Shuqi Xu, Xiaoxing Xia, Juergen Biener, Hartmut Haeffner, and Kristin Beck. "3D-printed ion traps for scalable quantum information processing." (Poster Presentation at American Physical Society (APS) Global Physics Summit 2025, Anaheim, California, March 2025). LLNL-POST-867742.

Parakh, Abhinav, Xiaoxing Xia, Sayan Patra, Adrian Guan, Juergen Biener, and Kristin M. Beck. "Making Miniature 3D Ion Traps with 3D Printing at LLNL." (Poster Presentation at Quantum Computing Program Review, College Park, MD, August 2025). LLNL-POST-2009512.

Guan, Adrian, Abhinav Parakh, Xiaoxing Xia, Sayan Patra, Kristin Beck, and Juergen Biener. 2025. "Miniaturized 3-D Printed Ion Traps for Quantum Computing." (Poster Presentation at PLS Summer Student Showcase, Livermore, CA, July). LLNL-POST-2008468.

Ainsworth, Rachel Leilani, Sayan Patra, and Kristin Beck. 2024. "Stabilizing Lasers to a High Finesse Wavelength Meter for laser cooling of 40Ca^+ ions." (Poster Presentation at LLNL SULI Poster Presentations, Livermore, CA, December). LLNL-POST-2001527.

Technical Reports

Ainsworth, Rachel Leilani, Sayan Patra, and Kristin Beck. 2024. "Implementing a laser stabilization system for trapping Ca⁺ ions: an internship reflection." Science Undergraduate Laboratory Internships (SULI) Final Report. LLNL-TR-871837.

Presentations

Kristin Beck. "3D-printed ion traps for reduced heating rates and rapid trap design." (Presented at IEEE Quantum Week, Montreal, CA, September 2024).

Hartmut Haeffner, Shuqi Xu, Xiaoxing Xia, Qian Yu, Bingran You, Merrell Brzeczek, Sean Buechele, Boerge Hemmerling, Andrew Jayich, Abhinav Parakh, Kristin Beck, Juergen Biener, 2024, "3D-Printed Micro Ion Trap Technology for Scalable Quantum Information Processing." (Presented at North American Conference on Trapped Ions, Los Angeles, California, August 2024).

Hartmut Haeffner. "3D-Printed Micro Ion Trap Technology for Scalable Quantum Information Processing." (Presented at RIKEN-LBNL Workshop on Quantum Information Science, Lawrence Berkeley National Laboratory, Berkeley, California, September 2024).

Shuqi Xu, Xiaoxing Xia, Qian Yu, Sumanta Khan, Eli Megidish, Bingran Yu, Merrell Brzeczek, Sean Buechele, Boerge Hemmerling, Andrew Jayich, Abhinav Parakh, Kristin Beck, Juergen Biener, Hartmut Haeffner, 2024, "3D-Printed Micro Ion Trap Technology for Scalable Quantum Information Processing." (Presented at 55th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, Fort Worth, Texas, June 2024).

Abhinav Parakh. "Additive Manufacturing for Quantum Computing." (Presented at LLNL Research SLAM!, LLNL, Livermore, California, September 2024).

Abhinav Parakh. "AM of ion traps for quantum computing." (Presented at Micro and Nano Technology Section Meeting, LLNL, Livermore, CA, May 2024).

Xiaoxing Xia. "Igniting the Future: Additive Manufacturing for Fusion Energy, Quantum Computing, and Neuromorphic Materials." (Presented at Army Research Office workshop on Next Generation Processing in Extreme Environments, Adelphi, Maryland, December 2023).

Andrew Jayich. "Ions for transportable optical clocks." (Presented at North American Conference on Trapped Ions, Los Angeles, California, August 2024).

Andrew Jayich. "Radium Clocks." (Presented at European Conference on Trapped Ions, Buckeburg, Germany, September 2023).

Kristin Beck. "Reducing Noise in Quantum Processors." (Presented at Physics Department Colloquium, University of California at Davis, Davis, California, November 2023).

Sayan Patra, 2025, "3D-printed ion traps for quantum applications." (Presented at American Physical Society (APS) Division of Atomic, Molecular and Optical Physics (DAMOP) Meeting 2025, Portland, Oregon, June 2025).

Kristin Beck. "3D-printed ion traps for quantum computing." (Presented at Society of Physics Students (SPS) Seminar, Stanislaus State, Turlock, California, April 2025).

Kristin Beck, "3D-printed ion traps for quantum computing." (Presented at Duke Quantum Center Seminar, Duke University, Durham, North Carolina, March 2025).

Andrew Jayich. "Heavy metal clocks." (Presented at University of California at Berkeley Atomic and Molecular Optics (AMO) seminar, Berkeley, California, September 2025).

Andrew Jayich. "Heavy metal optical clocks." (Presented at Georgia Tech/Georgia Tech Research Institute Atomic and Molecular Optics (AMO) Seminar, Atlanta, Georgia, February 2025).

Xiaoxing Xia. "Igniting the future through high-precision, high-throughput additive manufacturing." (Presented at 2025 American Chemical Society (ACS) Spring Meeting, San Diego, California, March 2025).

Adrian Guan. "Miniaturized 3-D Printed Ion Traps For Quantum Applications." (Presented at Livermore Center for Quantum Science Intern Capstone Presentations, Livermore, California, July 2025).

Hartmut Haeffner. "Quantum Computing and Information with 3D Printed Ion Traps." (Presented at UC Noyce Symposium, Irvine, California, October 2024).

Andrew Jayich. "Transportable optical clocks to search for new physics." (Presented at Physics of Quantum Electronics 2025, Snowbird, Utah, January 2025).

Records of Invention

Beck, Kristin, Juergen Biener, Abhinav Parakh, and Xiaoxing Xia. 2024. "Miniaturized Ion Traps on Heterogeneous Microchips." 2025-022.

Parakh, Abhinav, and Xiaoxing Xia. 2025. "Three-Dimensional Micro Junction Array Decoration of a Surface Electrode Ion Trap for Stable Ion Trapping and Transport." 2025-293.

23-ERD-022: Localizing and Explaining Performance Defects in Heterogeneous Applications

Project Overview

Performance defects are easy to introduce in scientific high performance computing (HPC) applications, which have deep software stacks and execute on a variety of heterogeneous hardware, but hard to find and fix. We propose an automated approach for detecting and fixing them both during the development process, for new applications, and post development, for existing ones, using sophisticated profiling and code mutation techniques.

In this work we researched and delivered tools and methods that automatically detect the root cause of performance defects and automatically apply these code fixes that resolve those defects. Specifically, the project's outcomes include methods and tools to: (1) extract code snippets from large applications and analyze them as independent executables. Perform automated code modifications in these snippets automatically and identify possible code modifications to these snippets that improve performance. Finally expose the performance improving modification to the user. A large part of the project focused on searching a combinatorial space of possible valid code modifications. To reduce our search time, we relied on Bayesian Optimization search algorithms, to stochastically focus our search to the modifications that are likely to have beneficial performance. This work publicly released the snippet extraction and snippet execution functionality to the LLVM. Finally, the project results were instrumental in proposing and receiving funding for two additional projects that use the findings of this project.

Mission Impact

HPC systems are critical infrastructure where advanced simulations are running to safeguard the NNSA stockpile, address DOE's energy and environmental security missions, and enhance the understanding of national security challenges to design effective responses. Executing those applications at the highest possible performance is paramount for efficacy and competitiveness. This project researched and developed fundamental computer science methods to improve the performance of HPC applications through automated system software technologies while also being one of the first projects to represent software development as a task applicable to machine learning research. The project disseminated research findings through numerous publications and presentations in top-tier venues to strengthen LLNL's leadership in this area of research while also organizing workshops in these topics. During the project, we formed and maintained strong collaborations with other national laboratories (Argonne National Laboratory), industry (AMD), academia (UMD), international universities (ETH) and the LLVM development community. Those collaborations enriched the research environment and transferred substantial expertise to LLNL.

Publications

Schaad, Philipp, Tal Ben-Nun, and Torsten Hoefler. 2025. "C.A.T.S.: Memory and Control Flow Tracing for Whole-Program Performance Analysis." In the Proceedings of Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, St. Louis, MO. LLNL-CONF-2003780.

Wu, Jianbo, Jie Ren, Shuangyan Yang, Konstantinos Parasyris, Giorgis Georgakoudis, Ignacio Laguna, and Dong Li. 2025. "LM-Offload: Performance Model-Guided Generative Inference of Large Language Models with Parallelism Control." In the Proceedings of 2025 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), Milan, Italy. LLNL-CONF-2004865.

Miao, Dolores, Ignacio Laguna, Giorgis Georgakoudis, Konstantinos Parasyris, and Cindy Rubio-González. 2024. "MUPPET: Optimizing Performance in OpenMP via Mutation Testing." In the Proceedings of Proceedings of the 15th International Workshop on Programming Models and Applications for Multicores and Manycores, Edinburgh, United Kingdom. <https://doi.org/10.1145/3649169.3649246>. LLNL-CONF-858593.

Georgakoudis, Giorgis, Konstantinos Parasyris, and David Beckingsale. 2025. "Proteus: Portable Runtime Optimization of GPU Kernel Execution with Just-in-Time Compilation." In the Proceedings of Proceedings of the 23rd ACM/IEEE International Symposium on Code Generation and Optimization, Las Vegas, NV, USA. <https://doi.org/10.1145/3696443.3708939>. LLNL-CONF-869329.

Parasyris, Konstantinos, Giorgis Georgakoudis, Esteban Rangel, Ignacio Laguna, and Johannes Doerfert. 2023. "Scalable Tuning of (OpenMP) GPU Applications via Kernel Record and Replay." In the Proceedings of Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, Denver, CO, USA. <https://doi.org/10.1145/3581784.3607098>. LLNL-CONF-847175.

Davis, Joshua Hoke, Pranav Sivaraman, Joy Kitson, Konstantinos Parasyris, Harshitha Menon, Isaac Minn, Giorgis Georgakoudis, and Abhinav Bhatele. 2025. "Taking GPU Programming Models to Task for Performance Portability." In the Proceedings of Proceedings of the 39th ACM International Conference on Supercomputing, Utah, USA. <https://doi.org/10.1145/3721145.3730423>. LLNL-CONF-2004865.

Laguna, Ignacio, Patrick Chapman, Konstantinos Parasyris, Giorgis Georgakoudis, and Cindy Rubio-González. 2024. "Testing the Unknown: A Framework for OpenMP Testing via Random Program Generation." In the Proceedings of SC24-W: Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis, Atlanta GA USA. LLNL-CONF-868411.

Presentations

Konstantinos Parasyris. "Escaping the Performance Portability Trap: A Case of re-arranging priorities." (Presented at International Workshop on Accelerators and Hybrid Emerging Systems (AsHES)., Milan, Italy, June 2025).

Giorgis Georgakoudis. "Investigating Just-In-Time (JIT) runtime optimizations using LLVM." (Presented at CASC Division Meeting, CASC, LLNL, March 2024).

Konstantinos Parasyris, 2024, "Localizing and Explaining Performance Defects in Heterogeneous Applications." (Presented at Intro to DOE's ASCR Program and the Early Career Award Process, CASC, LLNL, June 2024).

Tal Ben-Nun, 2024, "Machine Learning for Performance Engineering Across Applications." (Presented at Machine Learning Support for the Lifetime of Software (ML4SW), Zurich, Switzerland, June 2024).

Konstantinos Parasyris, 2024, "Scalable Tuning of (OpenMP) GPU Applications via Kernel Record and Replay." (Presented at CASC, Division Meeting, CASC, LLNL, May 2024).

Konstantinos Parasyris, 2023, "Scalable Tuning of (OpenMP) GPU Applications via Kernel Record and Replay." (Presented at The International Conference for High Performance Computing, Networking, Storage, and Analysis, Dallas, US, November 2023).

Code

Ben-Nun, Tal, and Konstantinos Parasyris. 2025. *ArgoCC*.

Ben-Nun, Tal. 2025. *C.A.T.S.: Memory and Control Flow Tracing for Whole-Program Performance Analysis*.

Parasyris, Konstantinos, and Giorgis Georgakoudis. 2024. *Mneme*. <https://github.com/Olympus-HPC/Mneme>.

Parasyris, Konstantinos, Giorgis Georgakoudis, Ignacio Laguna Peralta, Cindy Rubio-Gonzalez, and Dolores Miao. 2024. *MUPPET: An automated OpenMP mutation testing framework for performance optimization*. <https://www.osti.gov/biblio/code-152898>.

Georgakoudis, Giorgis, and David Beckingsale. 2024. *Proteus*. <https://github.com/Olympus-HPC/proteus>.

23-ERD-025: Optimal Uses of Magnetic Fields for Indirect-Drive Inertial Fusion

Project Overview

This project explored how applied magnetic fields can improve inertial confinement fusion (ICF), specifically the indirect-drive approach that uses a hohlraum. This has been proposed for several decades as potentially beneficial, due to thermal insulation (reduced losses) from the imploded hotspot. We performed the most advanced radiation-magneto-hydrodynamic modeling to date of magnetized ICF designs in the ignition regime. We found that adding technologically feasible fields up to 60 – 70 Tesla could increase the fusion yield of current igniting designs for the National Ignition Facility (NIF) by up to 8x. Also, simulations show that in certain cases relatively small fields of 3 – 5 Tesla could double the yield, and be implemented at much lower cost. Early work on re-optimizing NIF designs with magnetic fields, namely by using a thicker ablator with more mass remaining, could increase the yield of a sub-ignition target by 18x and bring it into the ignition regime. A separate benefit of magnetization besides reduced thermal loss is reduced hydrodynamic instability. Modeling work under this project shows this could be significant, though early experiments at NIF and the Omega Laser proved inconclusive. We designed and proposed an improved NIF experiment on magnetized mix, based on a large-amplitude imposed perturbation. The project also supported basic physics research into magnetized laser-plasma interactions, namely cross-beam energy transfer, both with experiments at Omega and theory / modeling.

This project has substantially advanced the understanding of magnetized ICF. It points the way toward both increased absolute yields on lasers like NIF, and more robust and reproducible performance by mitigating degradations. This could be achieved by optimizing enhanced performance from thermal insulation with improved stability. Although future work is needed to better quantify these benefits of magnetization they directly support the goals of the ICF program (higher yield) and the HED program's mission to develop ignition applications (more reproducible yield).

Mission Impact

Our project advanced understanding of the potential benefits of magnetic fields to ICF ignition, for the stockpile stewardship, high-energy-density (HED) physics and fusion energy missions. Simulations showed that imposed fields can increase the fusion yield of existing NIF ignition designs, and that re-optimizing a non-igniting target can cause it to ignite. Obvious future work is to re-optimize the ignition designs with external magnetization. The main scientific next step for magnetized ICF is to test it on a NIF ignition target, but the facility does not currently have the capability to magnetize cryogenic targets. Our simulation finding that substantial magnetic yield enhancement could occur for low ~ 5 T field, as opposed to the 30 – 60 T previously contemplated, could greatly reduce the implementation cost on NIF. Magnetized ICF has additional non-technical benefits of being an innovative scientific topic and an excellent vehicle for LLNL to recruit and retain top scientists. NIF is currently the only facility in the world that can study magnetized burning plasmas, which is of interest to the NNSA as well as private fusion companies pursuing magnetized ICF or magneto-inertial fusion schemes.

Publications

Strozzi, D., H. Sio, G. Zimmerman, J. Moody, C. Weber, B. Djordjevic, C. Walsh, B. Hammel, B. Pollock, A. Povilus, J. Chittenden, and S. O'Neill. 2024. "Design and Modeling of Indirectly-Driven Magnetized Implosions on the NIF." *Physics of Plasmas* 31: 092703. <https://doi.org/10.1063/5.0214674>. LLNL-JRNL-862854.

Walsh, C., D. Strozzi, B. Pollock, B. Appelbe, A. Crilly, S. O'Neill, C. Weber, J. Chittenden, and J. Moody. 2024. "Resistive diffusion in magnetized ICF implosions: Reduced magnetic stabilization of the Richtmyer–Meshkov instability." *High Energy Density Physics* 51: 101103. <https://doi.org/10.1016/j.hedp.2024.101103>. LLNL-JRNL-856209.

O'Neill, S., B. Appelbe, A. Crilly, C. Walsh, D. Strozzi, J. Moody, and J. Chittenden. 2025. "Burn propagation in magnetized high-yield inertial fusion." *Physics of Plasmas* 32, no. 2 (February): 022703. <https://doi.org/10.1063/5.0242215>. LLNL-JRNL-868907.

Spiers, R., A. Bose, C. Frank, B. Lahmann, J. Moody, H. Sio, and D. Strozzi. 2025. "Hot-spot model for inertial confinement fusion implosions with an applied magnetic field." *Physics of Plasmas* 32, no. 7 (July): 072712. <https://doi.org/10.1063/5.0268309>. LLNL-JRNL-865615.

Walsh, C., S. O'Neill, D. Strozzi, L. Leal, R. Spiers, A. Crilly, B. Pollock, H. Sio, B. Hammel, B. Djordjevic, O. Hurricane, J. Chittenden, and J. Moody. 2025. "Magnetized ICF implosions: Ignition at low laser energy using designs with more ablator mass remaining." *Physics of Plasmas* 32, no. 7 (July): 072715. <https://doi.org/10.1063/5.0274275>. LLNL-JRNL-2011845.

Walsh, C., D. Strozzi, A. Povilus, S. O'Neill, L. Leal, B. Pollock, H. Sio, B. Hammel, B. Djordjevic, J. Chittenden, and J. Moody. 2025. "Magnetized ICF implosions: non-axial magnetic field topologies." *Nuclear Fusion* 65, no. 3 (February): 036040. <https://doi.org/10.1088/1741-4326/adb7f0>. LLNL-JRNL-871095.

Posters

Shi, Y. "Benchmarking Magnetized Three-Wave Coupling for Laser Backscattering." (Poster Presentation at American Physical Society Division of Plasma Physics, Denver, CO, October 2023). LLNL-CONF-856504.

Leal, L. "HYDRA Simulations Modeling Magnetized CBET Gas-Jet Experiments at OMEGA." (Poster Presentation at Anomalous Absorption Conference, Big Sky, MT, June) 2024. LLNL-POST-865235.

Djordjevic, B. "Integrated hohlraum simulations of magnetized burning plasmas." (Poster Presentation at NIF User Group Meeting, Livermore, CA, January 2024). LLNL-POST-859153.

Spiers, R. "Modeling Mix in ICF Implosions on the NIF With an Applied Magnetic Field." (Poster Presentation at LLNL summer student poster session, Livermore, CA, August) 2024). LLNL-POST-867356.

Pollock, B. "Status of the Magnetized Cross Beam Energy Transfer (MagCBET) Campaign." (Poster Presentation at Anomalous Absorption Conference, Big Sky, MT, June 2024). LLNL-CONF-865394.

Moody, J. "Thomson Scattering from a Magnetized CBET Experiment." (Poster Presentation at Anomalous Absorption Conference, Big Sky, MT, June 2024). LLNL-POST-856514.

Strozzi, David. "Exploring Axial and Other Imposed Magnetic Fields to Improve Layered Hohlraum-Driven Implosions." (Poster Presentation at Inertial Fusion Sciences and Applications, Denver, CO, USA, September 2024). LLNL-CONF-854882.

Moody, John. "Initial experimental results on magnetized cross-beam energy transfer." (Poster Presentation at APS Div. Plasma Physics 2024, Atlanta, GA, October) 2024). LLNL-POST-870085.

Djordjevic, Blagoje. "Integrated Radiation-Magneto-Hydrodynamic Simulations of Magnetized Burning Plasmas." (Poster Presentation at NIF User Group meeting, Livermore, CA, February 2025). LLNL-PRES-865314.

Djordjevic, Blagoje. "Integrated Radiation-Magneto-Hydrodynamic Simulations of Magnetized Igniting Plasmas." (Poster Presentation at Anomalous Absorption Conference 2025, Sedona, AZ, May 2025). LLNL-POST-2006026.

Djordjevic, Blagoje. "Integrated Radiation-Magneto-Hydrodynamic Simulations of Magnetized Igniting Plasmas." (Poster Presentation at European Physical Society Plasma Meeting, Vilnius, Lithuania, July 2025). LLNL-POST-2007879.

Dow, Melissa. 2024. "Laser Scattering From Magnetized Plasma." (Poster Presentation at APS Four Corners Meeting, Flagstaff, AZ, October). LLNL-POST-870870.

Shi, Yuan. 2024. "Status of the magnetized cross beam energy transfer (MagCBET) campaign." (Poster Presentation at APS Div. Plasma Physics 2024, Atlanta, GA, October). LLNL-CONF-865394.

Presentations

C. Walsh. "Application of Non-Uniform Magnetic Fields to Inertial Confinement Fusion Implosions." (Presented at American Physical Society Division of Plasma Physics, Denver, CO, October 2023).

D. Strozzi. "Finding the Best Uses of Imposed Magnetic Fields to Improve Indirect Drive Inertial Confinement Fusion." (Presented at American Physical Society Division of Plasma Physics, Denver, CO, October 2023).

B. Djordjevic. "Integrated Radiation-Magneto-Hydrodynamic Simulations of Magnetized Burning Plasmas." (Presented at Anomalous Absorption Conference, Big Sky, MT, June 2024).

John Moody, 2025, "Direct and indirect effects from magnetized cross-beam energy transfer." (Presented at Inertial Fusion Sciences and Applications, Tours, France, September 2025).

Blagoje Djordjevic. "Integrated Radiation-magneto-hydrodynamic Simulations of Magnetized Burning Plasmas." (Presented at Symposium and Summer School on Physics of Ionized Gases, Belgrade, Serbia, August 2024).

Blagoje Djordjevic. "Integrated radiation-magneto-hydrodynamic simulations of magnetized burning plasmas." (Presented at APS Div. Plasma Physics 2024, Atlanta, GA, October 2024).

B. Pollock, "Magnetized crossbeam energy transfer (MagCBET) PIC simulations and OMEGA experiments." (Presented at Anomalous Absorption Conference 2025, Sedona, AZ, May 2025).

Chris Walsh, "Magnetized ICF implosions: ignition at lower laser energy using designs with more mass remaining ." (Presented at Inertial Fusion Sciences and Applications, Tours, France, September 2025).

Robert Spiers "Modeling of Magnetized-ICF Experiments at the NIF." (Presented at APS Div. Plasma Physics 2024, Atlanta, GA, October 2024).

John Moody. "New effects from magnetized cross-beam energy transfer." (Presented at Anomalous Absorption Conference 2025, Sedona, AZ, May 2025).

23-ERD-026: High-Order General-Discrete-Ordinates Method Enabling Efficient Deterministic Transport in Hydrodynamic Simulations

Project Overview

Deterministic transport simulations for national-security and energy applications often operate in high-dimensional phase-space, where accuracy and cost both become major challenges. A common numerical artifact in such problems is the “ray-effect,” which appears as unphysical streaks. Beyond misinterpretation, these artifacts can contaminate tightly coupled physics, such as fluid dynamics, radiation-hydrodynamics, and laser-plasma interactions, eroding the predictive capability of entire multiphysics workflows. Our objective was to make high-dimension studies practical on modern hardware while mitigating the ray-effect without relying on prohibitively expensive sampling approaches such as Monte Carlo methods.

We developed the Generic Discretization Library (GenDiL), a Graphics Processing Unit (GPU)-first framework that uses high-order Discontinuous Galerkin (DG) methods and matrix-free algorithms to reduce memory usage and improve computational efficiency, critical for phase-space simulations. GenDiL supports phase-space adaptivity in both mesh size and polynomial order (hp-adaptivity) to place resolution only where it is needed. A central capability is Local Dimensional Refinement (LDR), which couples lower-dimension continuum models to higher-dimension kinetic models through stable and conservative interfaces, so that high-fidelity physics is applied only in regions where it is essential. Building on the GenDiL framework, we developed the General SN (GSN) family of algorithms as a true generalization of the polar SN approach (discrete ordinates, often denoted SN). Rather than tying discrete ordinates to a specific polar change of coordinates, GSN formulates transport on an arbitrary change of coordinates chosen to reduce ray-effect. We studied two complementary variants: an analytic variant, where the coordinate map is prescribed in advance by a closed-form function; and a data-driven variant, where a quantity of interest, such as the net flux, guides the coordinate system. GenDiL provides the library infrastructure for efficient GPU execution, but the GSN concept is algorithmic and independent of any one library. Across representative high-dimension tests, including non-symmetric solutions, both variants delivered strong ray-effect mitigation at practical cost, moving four- to six-dimensional analysis toward repeatable, routine studies.

Mission Impact

This work advances Lawrence Livermore National Laboratory (LLNL) missions by improving predictive simulation capabilities for transport and kinetic problems that underpin stockpile stewardship, inertial confinement fusion, and related multiphysics workflows. By combining Graphics Processing Unit (GPU)-first, matrix-free Discontinuous Galerkin methods with Local Dimensional Refinement and General SN coordinate strategies, the project enables higher accuracy per unit cost and practical reduction of ray-effect in deterministic simulations. By reducing artifact propagation into coupled models, the approach improves end-to-end predictive capability for mission-critical multiphysics simulations. The results are relevant to the Department of Energy and the National Nuclear Security Administration (DOE and NNSA) and generalize to other federal agency needs that depend on high-fidelity modeling. The work is already influencing the Laboratory

ecosystem through preparation of arbitrary-dimension abstractions for upstreaming into the RAJA performance library, interoperability with the MFEM finite-element library, and delivery of a kinetics mini-application (REVEMUP) used with an external partner in laser-plasma instability studies.

Software

Dudouit, Yohann, Holec, Milan, and Rotem, Amit Y. 2025. “Generic Discretization Library.” Computer software, February 3, 2025. <https://github.com/GenDiL/GenDiL>. <https://doi.org/10.11578/dc.20250507.2>.

Conference Presentations

Dudouit, Yohann, Holec, Milan, Rotem, Amit, Dobrev, Veselin, and Ricketson, Lee. “Advancing high-dimensional physics with matrix-free Discontinuous Galerkin methods.” In ICOSAHOM 2025.

Dudouit, Yohann, Dobrev, Veselin, Haut, Terry, Holec, Milan, Loffeld, John, Nikl, Jan, Ricketson, Lee, and Rotem, Amit. “A Matrix-Free High-Dimensional DG Approach for Mitigating the Rays-Effect in Phase-Space Advection.” In MFEM Workshop 2024.

Dudouit, Yohann, Dobrev, Veselin, Haut, Terry, Holec, Milan, Loffeld, John, Ricketson, Lee, and Rotem, Amit. “Mitigating the curse of dimensionality: Matrix-free high-order Discontinuous Galerkin methods for advection in phase space.” In NAHOMCon24, 2024.

Dudouit, Yohann, Dobrev, Veselin, Haut, Terry, and Holec, Milan. “Efficient high-dimension high-order matrix-free Discontinuous Galerkin methods for high-fidelity physics.” In ICOSAHOM 2023.

Dudouit, Yohann, Dobrev, Veselin, Haut, Terry, and Holec, Milan. “Efficient high-dimension high-order matrix-free Discontinuous Galerkin methods for high-fidelity physics.” In CEED 7th Annual Meeting, Sept. 2023.

23-ERD-027: Dual-Wavelength, Two-Photon Polymerization

Project Overview

In late 2022, the National Ignition Facility (NIF) achieved a major breakthrough by demonstrating controlled fusion through inertial confinement fusion (ICF), marking the first time that the energy produced by burning fusion plasma exceeded the energy required to initiate the reaction—a milestone known as scientific breakeven. Since then, NIF has achieved ignition multiple times, driving increased public and private investment in inertial fusion energy (IFE) as a clean, virtually limitless power source. However, transitioning ICF technology to practical IFE power plants requires significant technical advances and innovations. This project addresses one key challenge: the fuel target. Today's ICF fuel targets are nearly perfect hollow spheres (capsules) containing a thin inner layer of deuterium-tritium (DT) ice fuel. These targets take months to produce and days to prepare for use at NIF, yet an IFE power plant will likely require 100,000 to 1,000,000 fuel targets per day. To address this challenge, we have developed additive manufacturing (AM, or 3D printing) techniques to produce fuel targets with inner foam liners that enable rapid wicking and distribution of liquid DT, paving the way for efficient, high-volume fueling in future fusion power plants.

Our project focused on advancing multiphoton lithography (MPL) as a key AM method for fabricating foam-lined capsules. We designed and built a novel MPL printer with two unique capabilities: (1) a tunable laser that enables printing with different colors, allowing selective activation of material components for spatially controlled doping or simultaneous printing of foam and solid structures from a single feedstock; and (2) we coupled circular stage movements to galvanometer scanning to facilitate capsule fabrication with minimal stitching defects. In addition to our custom system, we leveraged commercial MPL printers to fabricate 3–4 mm diameter, fuel capsules with low-density AM-lattice foams and developed the necessary handling, metrology, and testing protocols to produce leak-tight fuel targets. Some of these capsules were fielded on NIF in direct-drive wetted-foam ICF experiments. Finally, we developed a cryogenic test station to monitor liquid deuterium filling of AM-foam lattices, informing on-going lattice and capsule design.

Mission Impact

This project substantially advanced LLNL's additive manufacturing (AM) capabilities for foam-lined ICF fuel capsules, directly supporting the Laboratory's Inertial Fusion Energy (IFE) Institutional Initiative and enhancing its Advanced Materials and Manufacturing core competency. Through the development of novel hardware - including a dual-wavelength MPL printer and a cryogenic wetting test station - the project has broadened expertise and opened new research directions. The team now supports multiple related ICF/IFE projects, both LDRD-funded and externally sponsored, with results that directly advance DOE/NNSA missions by enabling scalable, rapid production of fuel capsules for fusion energy applications. Ongoing work, including NIF experiments planned for 2026 and beyond, continue to validate AM approaches and drive progress toward the high-volume capsule fabrication rates essential for future IFE power plants.

Publications, Presentations, and Patents

Brenda, L. G.-D.; Hitchcock, D.; Larsen, G., et al. 2023. "The Softer Side of Fusion Materials Development." *Advanced Materials & Processes* 181 (6): 12-16A.
<https://doi.org/10.31399/asm.amp.2023-06.p012>

Kemp, G. E., Bhandarkar, S., Blue, B. E., et al. "First Demonstration of a layered directed drive inertial confinement fusion target on the National Ignition Facility." Presentation, 13th International Conference on Inertial Fusion Sciences and Applications, Tours, France, September 14-19, 2025.

Kemp, G. E., Yeamans, C. B.; Hohenberger, M. et al. 2025. "Exploration of polar direct drive wetted foam concepts for neutron sources on the National Ignition Facility Laser." *Physics of Plasma* 32: 022702. doi: 10.1063/5.0233748.

Moestopo, W. P. et al. 2025 "Fully Additive Manufactured Wetted Foam Capsules for Inertial Confinement Fusion." *Fusion Science and Technology Special Issue 25th Target Fabrication Specialist Meeting*. Under Review.

Moestopo, W. P. "Fully Additive Manufactured Wetted Foam Capsule for Inertial Confinement Fusion." Presentation, 2025 IFE-Star Conference, Breckenridge, CO, April 7-11, 2025.

Moestopo, W. P., Mettry-Yassa, M.; Schwartz, J. J. et al. "Fully additively manufactured wetted foam capsules for inertial confinement fusion." Presentation, 25th Target Fabrication Specialist Meeting, San Diego, CA, August 24-28, 2024.

Moestopo, W. P. "Hierarchical Micro-architected Materials." Presentation, UpNano Customer Event 2023, Vienna, Austria, June 21-23, 2023.

Xia, Xiaoxing. Kemp, G. E., Mariscal, D., et al. "Polar-direct-drive DT wetted foam studies on the National Ignition Facility." Presentation, 2025 IFE-STAR Summit, Breckenridge, CO, April 7-11, 2025.

Xia, Xiaoxing. "Igniting the future through high-precision, high-throughput additive manufacturing." Invited presentation, 2025 American Chemical Society Spring Meeting, San Diego, CA, March 23-27, 2025.

23-ERD-028: Novel Pathways for Storing Energy

Project Overview

The motivations for this project were: (1) to predict novel high energy density materials (HEDM) using first principles theory and evaluate their energetic performance by thermochemical calculation, and (2) to establish a technologically up-to-date reaction propagation rate (RPR) experimental capability for rapid evaluation of known and novel HEDMs. The project has used state-of-the art theoretical approaches to evaluate HEDM candidate molecules and mixtures and has seen the construction and successful testing of a new RPR apparatus for the detailed investigation of explosives kinetics and chemistry at pressures relevant to deflagration and detonation.

Mission Impact

The LLNL mission and focus areas relevant to this project include High Explosives Physics, Chemistry and Materials, High Performance Computing Simulation and Data Science, and Accelerated Materials and Manufacturing. The project has seen the application of state-of-the art theoretical approaches to predict the formation of potential novel energetic materials from candidate precursor molecules and mixtures. A modern RPR capability has been developed which allows testing of HEDM and that requires only microscopic quantities of material (thus without the traditional safety and cost concerns of larger scale conventional tests). This is very desirable not only for testing novel HEDM but providing insight into persistent questions regarding the chemistry and kinetics of otherwise well-known high explosives. Such insight is expected to help accelerate a new generation of HEDMs with improved performance, reliability, and safety and as such contribute to maintaining and enhancing the safety, security, and effectiveness of the U.S. nuclear weapons stockpile.

Publications

Steele, Brad A., Chris Perreault, Jason Baker, Huy Pham, and Jonathan Crowhurst. 2025. "Experimental and theoretical investigation into the high pressure deflagration products of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105)." *Combustion and Flame*, 275, 114067. <https://doi.org/10.1016/j.combustflame.2025.114067>.

Perreault, Christopher, Jason Baker, and Jonathan Crowhurst. 2025. "Two-dimensional burn velocity and analysis of burn products of nitromethane at high pressure." *Combustion and Flame*, 280, 114348. <https://doi.org/10.1016/j.combustflame.2025.114348>.

Ahmad, Rasool, Jonathan Crowhurst, and Stanimir Bonev. 2025. "Photo-induced electronic excitations drive polymerization of carbon monoxide: A first-principles study." *Journal of Chemical Physics*, accepted.

Paul, Reetam, Jonathan C. Crowhurst, and Stanimir A. Bonev. 2025. "Prediction of an alternative route to polymeric carbon dioxide: A metastable energetic material." *Communications Chemistry*, accepted.

Presentations

Paul, Reetam, 2024. "Prediction of Pressure-induced Polymerization and Recovery of a Dense and Energetic CO-O₂ Phase", APS March Meeting 2024, March 3-8, 2024, Minneapolis, Minnesota.

Paul, Reetam, 2024. "Pressure-induced polymerization and chemical hysteresis in metastable mixtures of molecular solids", Gordon Research Seminar 2024, July 13-19, 2024, Holderness, New Hampshire.

J. C. Crowhurst, 2024. "Inferring macroscopic properties of high explosives by analyzing burn behavior in microscopic samples", Crowhurst et al, 2024 JOWOG 9 Initiation Train Meeting, May 14-16, 2024, Lawrence Livermore National Laboratory.

Perreault, C. 2025 "Two-Dimensional Burn Velocity and Analysis of Burn Products of Nitromethane at High Pressure", Poster. APS SCCM Meeting 2025: 24th International Conference on the Science of Compression in Condensed Matter, June 22-27, 2025, Washington, DC.

23-ERD-029: Knowledge Extraction and Injection Via Concept-Level Reasoning in Scientific Machine Learning

Project Overview

Scientific discovery increasingly relies on machine learning (ML) models to analyze complex data and generate predictions that push the boundaries of knowledge. However, the opaque nature of deep learning models limits their usefulness in scientific domains, where understanding and trust in model reasoning are essential. This LDRD project is motivated by the need to create a shared language that connects ML models with their users. Overall, this LDRD approaches the challenge of human-AI interaction from two complementary perspectives: making concepts explicit within models and facilitating more effective translation of user intentions to machines. In the first direction, we develop novel approaches to discover domain concepts in scientific ML models and methods to reason about predictions through intervention using these concepts. This empowers scientists to interpret, trust, and guide machines, ultimately enabling more informed decision-making and accelerating scientific discovery. In the second direction, we leverage human-in-the-loop model steering to facilitate direct injection of user knowledge into predictive models, as well as LLM agents that can translate user intentions into tangible machine instructions to facilitate intuitive scientific workflows. Through both avenues, we facilitate more effective communication and knowledge exchange between humans and AI.

Mission Impact

The outcome of the project fills an essential need in scientific machine learning by establishing a standardized framework for identifying and reasoning about domain-specific concepts within data-driven models. By making these concepts explicit and actionable, we bridge the gap between machine learning models and domain users, ultimately fostering greater trust, interpretability, and guidance in AI-driven discovery. For example, our web-based, human-in-the-loop segmentation tool for scanning electron microscopy (SEM) images in materials science, deployed on LC container servers, has already demonstrated practical value in real-world research workflows. Our novel concept discovery methods, such as using sparse autoencoders, enable us to identify and control representations of critical phenomena like vortex phases in the latent spaces of computational fluid dynamics (CFD) models. Furthermore, by generating material images conditioned on attributes discovered within model representations, we enable targeted exploration and hypothesis testing in materials science. Our approach also supports concept-aware comparisons of complex datasets, facilitating the exploration of similarities and differences between experimental and simulation-based models. To lower the barrier to entry for advanced scientific data analysis, we have developed agentic tools that translate user language instructions into concrete actions within established platforms such as *ParaView* for volumetric data and *napari* for bio-SEM images. These tools empower scientists to directly translate scientific intent into actionable workflows. By demonstrating these capabilities across mission-critical applications, including materials science, high-energy-density physics, and computational fluid dynamics, this project delivers foundational tools and methodologies that will enable the scientific community to meet future national security and technological challenges.

Publications and Presentations

Jeong, Sangwon, Mingwei Li, Matthew Berger, and Shusen Liu. 2023. "Concept Lens: Visually Analyzing the Consistency of Semantic Manipulation in GANs." In 2023 IEEE Visualization and Visual Analytics (VIS), pp. 221-225. IEEE. LLNL-CONF-848581

Jeong, Sangwon, Jixian Li, Christopher Johnson, Shusen Liu, and Matthew Berger. 2024. "Text-based Transfer Function Design for Semantic Volume Rendering." In the Proceedings of IEEE Visualization Conference, St. Pete Beach, Florida, USA. LLNL-CONF-863784.

Berger, Matthew, and Shusen Liu. 2024. "The Visualization JUDGE: Can Multimodal Foundation Models Guide Visualization Design Through Visual Perception?" In the Proceedings of IEEE Visualization Conference, BELIV workshop, St. Pete Beach, Florida, USA.. LLNL-PROC-866816.

Liu, Shusen, Haichao Miao, Zhimin Li, Matthew Olson, Valerio Pascucci, and Peer-Timo Bremer. 2024. "AVA: Towards Autonomous Visualization Agents through Visual Perception-Driven Decision-Making." Computer Graphics Forum. LLNL-CONF-857838.

Li, Mingwei, Sangwon Jeong, Shusen Liu, and Matthew Berger. 2024. "CAN: Concept-Aligned Neurons for Visual Comparison of Deep Neural Network Models." Computer Graphics Forum. <https://doi.org/10.1111/cgf.15085>. LLNL-CONF-764021.

Li, Zhimin, Shusen Liu, Xin Yu, Bhavya Kailkhura, Jie Cao, James Daniel Diffenderfer, Peer-Timo Bremer, and Valerio Pascucci. 2024. "Understanding Robustness Lottery: A Geometric Visual Comparative Analysis of Neural Network Pruning Approaches." IEEE Transactions on Visualization and Computer Graphics (IEEE TVCG), LLNL-CONF-764021

Ai, Kuangshi, Haichao Miao, Zhimin Li, Chaoli Wang, and Shusen Liu. 2025. "An Evaluation-Centric Paradigm for Scientific Visualization Agents." In the Proceedings of Workshop on GenAI, Agents, and the Future of VIS (IEEE VIS), Vienna, Austria. LLNL-CONF-2010304.

Hu, Yeping, and Shusen Liu. 2025. "Interpreting CFD Surrogates through Sparse Autoencoders." In the Proceedings of Workshop on Explainable Artificial Intelligence (XAI) at the 34th International Joint Conference on Artificial Intelligence (IJCAI), Montreal, Canada. LLNL-CONF-2006343.

Liu, Shusen, Haichao Miao, and Peer-Timo Bremer. 2025. "ParaView-MCP: An Autonomous Visualization Agent with Direct Tool Use." In the Proceedings of IEEE Visualization Conference: Short Papers, Vienna, Austria. LLNL-CONF-2005387.

Yan, Xinyuan, Shusen Liu, Kowshik Thopalli, and Bei Wang Phillips. 2025. "Visual Exploration of Feature Relationships in Sparse Autoencoders with Curated Concepts." In the Proceedings of NeurIPS 2025 Workshop on Mechanistic Interpretability (MechInterp), San Diego, US, August. LLNL-CONF-2010620.

Jeong, Sangwon, Mingwei Li, Matthew Berger, and Shusen Liu. 2025. "Concept Lens: Visual Comparison and Evaluation of Generative Model Manipulations." IEEE Transactions on Visualization and Computer Graphics (IEEE TVCG). LLNL-JRNL-2011826.

Shusen Liu, Ruben Glatt, 2023, "Towards Micro-Structure Image Segmentation with No Training Data." (Presented at MSD Seminar (LLNL), B235 R1090, LLNL, November 2023).

Sangwon Jeong, 2023, "Concept Lens: Visually Analyzing the Consistency of Semantic Manipulation in GANs." (Presented at IEEE Visualization and Visual Analytics (VIS), 2023, IEEE).

Sangwon Jeong, 2024, "Text-based Transfer Function Design for Semantic Volume Rendering." (Presented at IEEE Visualization Conference, St. Pete Beach, Florida, USA, 2024).

Matthew Berger, 2024, "The Visualization JUDGE: Can Multimodal Foundation Models Guide Visualization Design Through Visual Perception?." (Presented at BELIV workshop, IEEE Visualization Conference, St. Pete Beach, Florida, USA, 2024).

Shusen Liu, 2024, "AVA: Towards Autonomous Visualization Agents through Visual Perception-Driven Decision-Making." (Presented at Computer Graphics Forum (CGF), 2024).

Mingwei Li, 2024, "CAN: Concept-Aligned Neurons for Visual Comparison of Deep Neural Network Models." (Presented at Computer Graphics Forum (CGF), 2024).

Shusen Liu, 2025, "ParaView-MCP: An Autonomous Visualization Agent with Direct Tool Use." (Presented at CASIS workshop, LLNL - UCLCC, April 2025).

Yeping Hu, 2025, "Interpreting CFD Surrogates through Sparse Autoencoders." (Presented at Workshop on Explainable Artificial Intelligence (XAI), IJCAI, Montreal, Canada, 2025).

23-ERD-030: ForwardProp: A Novel, Gradient-Free Learning Paradigm for Integrating Deep Neural Nets with Scientific Simulations

Project Overview

Scientific simulations are often prohibitively expensive, limiting the pace of scientific discovery. Machine learning (ML) offers the potential to accelerate and improve these simulations, but existing ML models struggle in complex domains due to large data requirements and limited ability to incorporate scientific knowledge. Current methods that integrate scientific knowledge into ML training require differentiable simulation codes, which are often unavailable or costly to develop.

In this project, we developed a novel general-purpose gradient-free ML training framework, called DeepZero, that enables the integration of scientific simulators with ML models without requiring gradient information. Unlike traditional gradient-based approaches, DeepZero trains ML models using only function queries, removing the need for auto-differentiation and making the method easy to adopt. This approach leverages zeroth-order optimization and architecture refinement to achieve high accuracy and generalization, comparable to differentiable physics methods, but with broader applicability. We coupled DeepZero with scientific simulation code PhiFlow and MFEM and built a data-generation pipeline for MFEM that can be used to generate data for training ML-based simulation correction models. This pipeline inherited some technology from the AMS SI, added new functionality specific to MFEM, and is robust enough to be used by future projects. We faced challenges with multiple layers of parallelism that were unforeseen when using Zeroth-order optimization for solver-in-the-loop simulation correction with non-differentiable simulation codes. In an effort to alleviate the burden of non-differentiable training, we considered various differentiable pretraining techniques that have potential to reduce non-differentiable training. To this end, we performed a study on adversarial robustness as we considered pretraining simulation correction functions using adversarial data. Further, after the initial success of DeepZero and the emergence of powerful LLMs and VLMs, we considered leveraging pretrained LLMs and VLMs to finetune as scientific ML models. This resulted in many studies on reasoning capabilities and hallucination issues which would be necessary to understand for scientific applications and robustness. While DeepZero allows for more accurate and faster simulations as an end product, the compute/overhead for training scientific-ML models with DeepZero is still a hinderance. While DeepZero is currently state-of-the-art for zeroth order optimization performance on popular benchmarks, our stretch goal of pushing efficiency further with new gradient estimators for DeepZero was still ongoing by the time the project concluded. Our project lays the foundation for a new class of ML-enhanced scientific workflows that are both flexible and high-performing.

Mission Impact

This research significantly advances LLNL's mission by providing new capabilities for integrating machine learning with scientific simulations, especially in high-performance computing (HPC), simulation, and data science. DeepZero's gradient-free training paradigm opens new research directions and supports rapid adoption of ML across a wide range of mission-critical applications. Further, we laid the foundation for new diffusion-based gradient estimation techniques that could improve both the efficiency and quality of DeepZero. Our work on reasoning benchmarking and

hallucination detection will be valuable in identifying how to meaningfully leverage LLMs and VLMs in scientific applications at LLNL. The project's outcomes are relevant to DOE/NNSA missions and other federal agencies by enabling more efficient, accurate, and generalizable scientific workflows, and by positioning LLNL as a leader in ML-driven simulation enhancement.

Publications

Bartoldson, Brian R., James Diffenderfer, Konstantinos Parasyris, and Bhavya Kailkhura. 2024. "Adversarial Robustness Limits via Scaling-Law and Human-Alignment Studies." In Proceedings of the 2024 International Conference on Machine Learning. Vienna, Austria.

Chen, Aochuan, Yimeng Zhang, Jinghan Jia, James Diffenderfer, Jiancheng Liu, Konstantinos Parasyris, Yihua Zhang, Zheng Zhang, Bhavya Kailkhura, and Sijia Liu. 2024. "DeepZero: Scaling up Zeroth-Order Optimization for Deep Model Training." In Proceedings of the 2024 International Conference on Learning Representations. Vienna, Austria.

Jia, Jinghan, Yihua Zhang, Yimeng Zhang, Jiancheng Liu, Bharat Runwal, James Diffenderfer, Bhavya Kailkhura, and Sijia Liu. 2024. "SOUL: Unlocking the Power of Second-Order Optimization for LLM Unlearning." In Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing, 4276–4292. Miami, Florida: Association for Computational Linguistics.

Ma, Shaocong, James Diffenderfer, Bhavya Kailkhura, and Yi Zhou. 2025. "Deep learning of PDE correction and mesh adaption without automatic differentiation." In *Machine Learning 114(3)*, 1-25.

Presentations

Diffenderfer, J. "DeepZero: Scaling up Zeroth-Order Optimization for Deep Model Training." Monterey Data Conference. Monterey, California. 2023.

Bartoldson, B. "Adversarial Robustness Limits via Scaling-Law and Human-Alignment Studies." 2024 International Conference on Machine Learning. Vienna, Austria, 2024.

23-ERD-031: Gallium-Arsenide Semiconductor Opening Switches for Pulsed-Power Systems

Project Overview

The goal of this work was to investigate design manufacturing semiconductor opening switches (SOS) in both silicon and gallium arsenide (GaAs). Solid-state opening switches are critical components for pulsed power systems and applications in directed energy, dielectric wall accelerators, and novel semiconductor manufacturing techniques. Under this funding, we have developed silicon SOS designs that suppresses an unwanted prepulse, increases the peak output voltage by about 10 percent, and reduces the pulse rise time by ~4x compared with more conventional profiles. Through this effort we have improved device fabrication and bonding techniques.

Additionally, work on this the GaAs opening switch has defined a unique application space that these devices are suited for. GaAs opening switches have short risetimes and pulse widths compared to silicon devices, however the short carrier lifetime of GaAs makes the circuit design more challenging than in silicon. For high PRF operation, the lifetime of the GaAs is an advantage compared to silicon. TCAD simulations of GaAs devices have been used to optimize a GaAs profile. Additionally, we have designed pulsers with sub 50ns reserve pump times and tested GaAs COTs PIN diodes in them.

Mission Impact

Work achieved under this LDRD has improved both the performance and manufacturability of silicon opening switches (SOS), directly advancing LLNL's mission in national security science and technology. SOS manufacturing techniques and device performance enable next generation pulsers that are strategic for multi domain deterrence in directed energy and pulsed power systems. This work is a key enabling technology for developing a dielectric wall accelerator (DWA), a platform with impact in both radiation therapy and strategic deterrence. Pulsers developed from these devices have also sparked early interest from the semiconductor manufacturing sector, including advanced lithography and plasma-based processing.

Through the successful delivery of devices to Sandia, the University of New Mexico, Texas Tech, and SARA Technologies for independent evaluation, this work has extended LLNL's reputation as a leader in semiconductor device development and pulsed power systems. The bases work helped to realize funding opportunities from the Air Force Research laboratory and the Joint Directed Energy Transition Office. These results reinforce partnerships across the NNSA, the Department of Defense, and academia, and have been substantial in closing capability gaps with China and Russia in these systems. Together, these impacts demonstrate that the project not only advances LLNL's core missions in national security and science, but also lays the groundwork for broader economic and technological benefits in the US industrial base.

Publications, Presentations, and Patents

C. A. Chapin, “High Voltage, Nanosecond Solid-State Switches,” presented at the DE Systems Symposium, Monterey, CA, Nov. 15, 2023. LLNL-PRES-856026.

C. A. Chapin, “Semiconductor Opening Switches: Semiconductors, Circuits, and Performance,” presented at the DE Systems Symposium, Monterey, CA, Nov. 20, 2024. LLNL-PRES-859292.

E. Schrock, Q. Shao, C. Chapin, J. Schrock, and L. Voss, “Evaluation and Optimization of Semiconductor Opening Switches,” presented at the Euro-Asian Pulsed Power Conference, Amsterdam Netherlands, Sept. 22, 2024. LLNL-ABS-862231.

C. A. Chapin *et al.*, “Solid State Switches for Pulsed Power Applications,” presented at the Government Microcircuit Applications & Critical Technology Conference, Defense Technical Information Center, Mar. 2024. LLNL-PRES-2003613. LLNL-CONF-860634.

Q. Shao, C. Chapin, S. E. Harrison, and L. F. Voss, “Semiconductor diode structures for pre-pulse elimination in switching or pulsing,” US20250374569A1.

C. A. Chapin *et al.*, “Dopant Optimization of Donors in Semiconductor Opening Switches to Eliminate Prepulse,” *IEEE Trans. Electron Devices*, vol. 72, no. 10, pp. 5496–5502, Oct. 2025, doi: 10.1109/TED.2025.3597885. LLNL-JRNL-2005999.

C. A. Chapin *et al.*, “Effect of Doping Profile on Silicon Semiconductor Opening Switch,” presented at the Government Microcircuit Applications & Critical Technology Conference, Defense Technical Information Center, Mar. 2025. doi: LLNL-PRES-2003613. LLNL-ABS-869357.

B. Esser *et al.*, “Testing of Novel Semiconductor Opening Switches Using Magnetic Switching,” *IEEE Trans. Plasma Sci.*, vol. 53, no. 8, pp. 1976–1981, Aug. 2025, doi: 10.1109/TPS.2025.3586185. LLNL-JRNL-2005563.

23-ERD-033: Nanoscale Precision Milling with Ion Beams

Project Overview

Recently introduced plasma focused ion beam (PFIB) technology could offer great flexibility and efficiency for the fabrication of laser target components. In order to effectively use PFIB with high precision and reproducibility, we need to develop detailed sets of process protocols based on the understanding of the physics and chemistry of ion-surface interactions. In this project, we studied how PFIB bombardment with different ion species (Xe, Ar, O, and N) interacts with prototypical carbon- and boron-based ablator materials (diamond and boron carbide) relevant to high-power laser targets and inertial confinement fusion. We quantified the ion beam milling rate and the resulting changes in the surface morphology as a function of several major process parameters, including ion mass, energy, incident beam angle, and gas-phase chemistry. Insights were applied to develop processes for drilling customized high-aspect-ratio holes - one of the key features of laser targets - in spherical diamond and boron carbide capsules.

Mission Impact

This project explores the science behind a method that helps position LLNL to address important emerging national needs and program growth. It expands the capabilities of precision target fabrication for ICF and HED programs. It also directly supports the Accelerated Materials and Manufacturing focus area, two Core Competencies (High Energy Density Science and Advanced Materials and Manufacturing), and the mission research challenge of nuclear weapon science.

Publications, Presentations, and Patents

Shin, S. J., Bayu Aji, L. B., Goodelman, D. C., Kim, E., Forien, J. B. and Kucheyev, S. O. 2024. "Precision milling of ablator materials with ion beams", 25th Target Fabrication Specialists Meeting, San Diego, CA, Aug 29. LLNL-PRES-867607

Shin, S. J., Goodelman, D. C., Bayu Aji, L. B., Forien, J. B., Kim, E., and Kucheyev, S. O. 2025. "Precision sputtering of diamond and boron carbide with plasma focused ion beams for high-aspect-ratio milling", Microscopy and Microanalysis 2025, Salt Lake City, UT, Jul 29. LLNL-CFPRES-2008669.

Shin, S. J. Forien, J. B., Goodelman, D. C., Bayu Aji, L. B., Kim, E., and Kucheyev, S. O. 2025. "Plasma focused ion beam milling of high-aspect-ratio holes in diamond", *Fusion Sci. Technol.*, published on-line. LLNL-JRNL-871745. <https://doi.org/10.1080/15361055.2025.2498198>.

Bayu Aji, L. B., Goodelman, D. C., Kim, E., Forien, J. B., Kucheyev, S. O., Shin, S. J. 2025. "Low-energy ion beam sputtering of polycrystalline diamond." LLNL-JRNL-2011327.

Goodelman, D. C., Kim, E., and Merlo, J. B. et. al. 2025. "Plasma focused ion beam sputtering of boron carbide." LLNL-JRNL-2011317.

23-ERD-034: An Integrated and Computational Approach to Optimization of Functionally-Graded Materials Using Additive Manufacturing

Project Overview

Many advanced technologies, such as next-generation energy systems, aerospace vehicles, and defense platforms, require materials that can withstand extreme environments, including high temperatures, corrosion, and radiation, while remaining strong and lightweight. Traditionally, joining different materials to achieve these properties introduces weak, failure-prone interfaces and defects that limit performance. Our research aimed to overcome this challenge by using additive manufacturing, specifically directed energy deposition, to create functionally graded materials—components with smooth transitions between different metals. This approach eliminates sharp boundaries and allows for tailored material properties throughout a part.

We combined advanced computational modeling with systematic experiments to design and fabricate these graded materials. Our team developed new software tools, such as the ESPEI, a path planner for optimizing compositional pathways between materials, and innovative methods for optimizing both the additive manufacturing process and post processing to start to produce components with quality approaching that of conventionally manufactured materials. We successfully produced and tested several new material gradients, including combinations of titanium, tantalum, niobium/C103, molybdenum/TZM, stainless steel, chromium, and other alloys. These functionally graded materials were evaluated through a wide range of tests, such as shock loading, high-temperature compression, gas gun impact, wind tunnel exposure, and advanced synchrotron imaging, many of which were applied to gradients for the first time. Our results demonstrate that it is possible to reliably manufacture and test these novel materials, revealing new insights into how multi-materials can be formed and perform, as well as providing a new axis for rapid materials exploration, and opening the door to using functionally graded materials as real, engineered solutions for demanding applications. This work represents a significant step forward in the design and deployment of multi-material components for extreme environments.

Mission Impact

This project significantly advances LLNL's national security mission by opening up material composition as a new degree of freedom in engineering design, fundamentally expanding the design space for critical components. Through the development of an integrated computational-experimental framework for rapid design and fabrication of functionally graded materials (FGMs), we provide LLNL and the NNSA complex with the unprecedented ability to design, qualify, and deploy multi-material solutions tailored for extreme environments and evolving mission needs. By enabling the creation of components with smoothly varying properties, this work directly supports programs focused on stockpile stewardship and advanced weapon system development, while also addressing urgent needs for novel or replacement materials—particularly those with vulnerable supply chains currently sourced from foreign suppliers or adversarial nations. The methodologies and tools developed here enhance the resilience and agility of the U.S. nuclear deterrent, expand the design space to include compositional gradients and novel alloy systems, and enable solutions for aging nuclear weapons systems. The impact of this work is further amplified through extensive

collaborations with industrial partners, academic institutions, and other national laboratories, accelerating technology transfer and ensuring rapid adoption of advanced materials and manufacturing techniques to meet mission needs across the DOE, NNSA, Department of Defense, and NASA. By fostering multidisciplinary collaboration and building expertise in advanced manufacturing and materials design, this project strengthens LLNL's leadership and positions the laboratory to support future mission-critical programs with innovative, resilient material solutions.

Publications

Ury, Nicholas, Brandon Bocklund, Aurelien Perron, and Kaila Bertsch. 2024. "Automated path planning for functionally graded materials considering phase stability and solidification behavior: Application to the Mo-Nb-Ta-Ti system." *Computational Materials Science*. <https://doi.org/10.1016/j.commatsci.2024.113172>. LLNL-JRNL-863614.

Bocklund, Brandon, Aurelien Perron, Joseph McKeown, and Kaila Bertsch. 2024. "Implementation of an extensible property modeling framework in ESPEI with applications to molar volume and elastic stiffness models." *Calphad*. <https://doi.org/10.1016/j.calphad.2024.102720>. LLNL-JRNL-XXXX.

Benjamin Ellyson, Brandon Bocklund, Jennifer Glerum, Nicholas Ury, Michael Juhasz, Raiyan Seede, Aurelien Perron, Kaila Bertsch. 2025. "Characteristic Length Scales and Microstructure Control through Post Processing of Additively Manufactured Ti-Ta Functionally Graded Materials." Under submission/review to *Acta Materialia*. LLNL-JRNL- 2011389.

Kaila Bertsch, Nicholas Ury, Brandon Bocklund, Benjamin Ellyson, Jennifer Glerum, Michael Juhasz, Aurelien Perron. 2025. "Evolution of microstructure in a Ti-Ta functionally graded material throughout the additive manufacturing process – Terminal melt pool analysis." Under submission/review. LLNL-JRNL- 2011971.

Posters

Bertsch, Kaila, Brandon Bocklund, Benjamin Ellyson, Jennifer Glerum, Michael Juhasz, and Aurelien Perron. 2025. "Design and Advanced Manufacturing of Novel Multi-Material Components with Compositional Gradients." (Poster Presentation at Conference Meeting, Washington D.C., May). LLNL-POST-2004701.

Juhasz, Michael, Brandon Bocklund, Benjamin Ellyson, Jennifer Glerum, Aurelien Perron, Nicholas Ury, Joseph McKeown, and Kaila Bertsch. 2025. "Design of Advanced Alloys and Functional Gradients with Directed Energy Deposition Additive Manufacturing." (Poster Presentation at Conference Meeting, Washington D.C., May). LLNL-POST-2004847.

Glerum, Jennifer, Benjamin Ellyson, Michael Juhasz, Brandon Bocklund, Nicholas Ury, Aurelien Perron, and Kaila Bertsch. 2025. "Integrated Computational-Experimental Framework for Additive Manufacturing of Functionally Graded Structural to Refractory Materials." (Poster Presentation at Conference Meeting, Los Alamos, New Mexico, USA, September). LLNL-POST-2009983.

Presentations

Nicholas Ury, Brandon Bocklund, Aurelien Perron, Kaila Bertsch, 2024, "Automated path planning for functionally graded materials considering phase stability and solidification behavior: Application to the Mo-Nb-Ta-Ti system." (Presented at The Minerals, Metals, and Mining Society Annual Meeting 2024, Orlando, FL, March 2024).

Raiyan Seede, Michael Juhasz, Jennifer Glerum, Benjamin Ellyson, Kaila Bertsch, 2024, "Enabling a Compositional Pathway from Titanium to Tantalum using Directed Energy Deposition." (Presented at The Minerals, Metals, and Mining Society Annual Meeting 2024, Orlando, FL, March 2024).

Jennifer Glerum, Benjamin Ellyson, Michael Juhasz, Raiyan Seede, Brandon Bocklund, Nicholas Ury, Aurelien Perron, Kaila Bertsch, 2024, "Functional Gradients in the Ti-Ta-Nb system." (Presented at Solid Freeform Fabrication Symposium, Austin, TX, August 2024).

Brandon Bocklund, Joseph McKeown, Aurelien Perron, Kaila Bertsch, 2024, "Implementation of an extensible property modeling framework in ESPEI." (Presented at Calphad, Mannheim, Germany, May 2024).

Benjamin Ellyson, Michael Juhasz, Raiyan Seede, Kaila Bertsch, 2024, "Thermo-Mechanical Performance of Compositionally Graded Refractory Alloys." (Presented at The Minerals, Metals, and Mining Society Annual Meeting 2024, Orlando, FL, March 2024).

Nicholas Ury, Benjamin Ellyson, Brandon Bocklund, Jennifer Glerum, Michael Juhasz, Aurelien Perron, Kaila Bertsch, 2025, "Design and Manufacturing of Defect-Free Functionally Graded Materials from Structural to Refractory Alloys." (Presented at Conference Meeting, Los Alamos, New Mexico, USA, September 2025).

Brandon Bocklund, Nicholas Ury, Benjamin Ellyson, Jennifer Glerum, Michael Juhasz, Aurelien Perron, Kaila Bertsch, 2025, "Implementation of an extensible property modeling framework in ESPEI with applications to molar volume and elastic stiffness models." (Presented at The Mining, Minerals, and Metals Society Annual Meeting 2025, Las Vegas, Nevada, March 2025).

Kaila Bertsch, Brandon Bocklund, Benjamin Ellyson, Jennifer Glerum, Michael Juhasz, Nicholas Ury, Aurelien Perron, 2025, "Integrated Computational-Experimental Framework for Production of AM Functionally Graded Materials From Structural to Refractory Alloys." (Presented at The Mining, Minerals, and Metals Society Annual Meeting 2025, Las Vegas, Nevada, March 2025).

Kaila Bertsch, Brandon Bocklund, Benjamin Ellyson, Jennifer Glerum, Michael Juhasz, Nicholas Ury, Aurelien Perron, 2025, "Integrated Computational-Experimental Framework for Production of AM Functionally Graded Materials From Structural to Refractory Alloys." (Presented at Solid Freeform Fabrication Symposium, Austin, Texas, August 2025).

Jennifer Glerum, Brandon Bocklund, Benjamin Ellyson, Michael Juhasz, Nicholas Ury, Aurelien Perron, Kaila Bertsch, 2025, "Production and Validation of Refractory Functionally Graded

Materials." (Presented at The Mining, Minerals, and Metals Society Annual Meeting 2025, Las Vegas, Nevada, March 2025).

Benjamin Ellyson, Brandon Bocklund, Nicholas Ury, Jennifer Glerum, Michael Juhasz, Aurelien Perron, Kaila Bertsch. "Thermal Stability of Functionally Graded Materials." (Presented at The Mining, Minerals, and Metals Society Annual Meeting 2025, Las Vegas, Nevada, March 2025).

23-ERD-035: Data-Driven Atomic Physics with High Repetition Rate Experiments

Project Overview

High-energy-density (HED) plasma experiments are essential for advancing atomic physics, fusion energy, and national security applications, but traditional approaches have been limited by slow data acquisition and manual analysis processes. This project addressed these challenges by developing a comprehensive suite of machine learning (ML) tools and frameworks specifically designed for high-repetition-rate (HRR) laser-driven plasma experiments. Our approach integrated multi-physics simulations, ML-driven experimental steering, and rapid diagnostic analysis to create a truly data-driven scientific workflow.

We developed ML-based analysis toolkits for spectroscopy, created surrogate models for atomic physics calculations that achieved approximately 10,000 times faster analysis than traditional methods, performed high-data-volume short-pulse high-intensity isochoric heating experiments with HRR spectrometers, and implemented autonomous control platforms for HRR experiments. These innovations enabled a greater than 10-fold increase in data throughput, allowing for real-time analysis and experimental guidance. We successfully demonstrated autonomous HRR experiments with direct ML-based control and developed empirical surrogate models validated by thousands of experimental datapoints. Our tools enabled rapid, accurate analysis of experimental spectra and real-time steering of plasma conditions to desired states, representing a paradigm shift in how HED science is conducted. This work has established a foundation for accelerated learning and improved model validation in laser-plasma experiments, with direct applications to fusion energy research and national security missions.

Mission Impact

The Data-Driven Atomic Physics project advances LLNL's Core Competencies in high-performance computing, simulation, and data science. By developing innovative ML tools and autonomous experimental platforms, we have enhanced the Laboratory's capabilities in several key areas. The use of ML surrogate models of kinetic-scale (particle-in-cell) physics to inform energy deposition in traditional radiation hydrodynamics simulations enables more accurate and computationally efficient modeling of HED plasmas. This directly supports LLNL's mission in stockpile stewardship by providing improved tools for predicting the behavior of materials under extreme conditions. Our autonomous experimental platforms dramatically increase the rate at which scientific data can be collected and analyzed, enabling rapid exploration of complex parameter spaces and accelerated discovery of new phenomena. This capability strengthens LLNL's position as a leader in scientific innovation and for the first time demonstrates the possibility of utilizing deep learning methods for achieving targeted plasma states that could be extended to more complex HRR HED systems. The ML-based analysis tools we developed enhance LLNL's ability to extract meaningful information from experimental data from HRR diagnostics in real-time, supporting multiple programmatic applications from fusion energy research to national security mission space. By pioneering the integration of ML with traditional physics simulations, this project reinforces LLNL's leadership in computational physics and advances the Laboratory's position at the forefront of scientific machine

learning. The ability to rapidly validate and refine atomic physics models is crucial for nuclear deterrence, nonproliferation, and emergency response applications, providing new capabilities for responding to emerging security challenges and advancing energy and environmental security missions.

Publications, Presentations, and Patents

Zeraouli, Ghassan, Derek Mariscal, Reed Hollinger, Sinah Zahedpour-Anaraki, Eric Folsom, Elizabeth Grace, Dean Rusby, Matthew Hill, Gerald Williams, Graeme Scott, Bryan Sullivan, Shoujun Wang, J King, Kelly Swanson, Raspberry Simpson, Blagoje Djordjevic, Scott Andrews, Rob Costa, Robert Cauble, Felicie Albert, Jorge Rocca, and Tammy Ma. 2023. "Flexible tape-drive target system for secondary high-intensity laser-driven sources." *Review of Scientific Instruments*. <https://doi.org/10.1063/5.0180715>. LLNL-JRNL-856290.

Zeraouli, Ghassan, Derek Mariscal, Kelly Swanson, Elizabeth Grace, Eric Folsom, Matthew Hill, Gerald Williams, Raspberry Simpson, Blagoje Djordjevic, Rebecca Daskalova, German Tiscareno, David Hanggi, Pedro Spingola, Brady Unzicker, Conrad Kuz, Scott Andrews, Rob Costa, Robert Cauble, Felicie Albert, Douglass Schumacher, Jorge Rocca, and Tammy Ma. 2024. "High repetition-rate dual-channel X-ray spectrometer for high-intensity laser-plasma experiments." *Review of Scientific Instruments*. <https://doi.org/10.1063/5.0217715>. LLNL-JRNL-868945.

Mariscal, Derek, Blagoje Djordjevic, Rushil Anirudh, Jay Jayaraman-Thiagarajan, Elizabeth Grace, Raspberry Simpson, Kelly Swanson, Tom Galvin, Daniel Mittelberger, John Heebner, Ryan Muir, Eric Folsom, Matthew Hill, Scott Feister, Emiko Ito, Keily Valdez-Sereno, Jorge Rocca, Jaebum Park, Shoujun Wang, Reed Hollinger, Ryan Nedbailo, Bryan Sullivan, Ghassan Zeraouli, Ankita Shukla, Pavan Turaga, Abhik Sarkar, Brian Van Essen, Shusen Liu, Brian Spears, Timo Bremer, and Tammy Ma. 2024. "Towards Machine-Learning-Assisted PW-class High-repetition-rate Experiments with Solid Targets." *Physics of Plasmas*. <https://doi.org/10.1063/5.0190553>. LLNL-JRNL-858036.

Eisenbach, S, D A Mariscal, R S Dorst, T Van Hoomissen, A M Ortiz, H Zhang, J J Pilgram, C G Constantin, L Rovige, P V Heuer, and others. 2024. "Machine learning analysis of high-repetition-rate two-dimensional Thomson scattering spectra from laser-produced plasmas." *Journal of Physics D: Applied Physics* 58, no. 3 (January): 035202. LLNL-JRNL-864719.

Djordjevic, B Z, J Kim, S C Wilks, J Ludwig, C Myers, A J Kemp, K K Swanson, G Zeraouli, E S Grace, R A Simpson, and others. 2023. "Transfer learning and multi-fidelity modeling of laser-driven particle acceleration." *Physics of Plasmas* 30, no. 4 (April). LLNL-JRNL-843173.

Djordjevic, Blagoje Z, and others. 2024. "Study of Thermalization Rates via Molecular Dynamics in Laser Driven High Energy Density Plasmas." In the Proceedings of LLNL Computing Grand Challenge Seminar, August, 2024. LLNL-PRES-868524.

Djordjevic, Blagoje Z, and others. 2023. "Transfer Learning and Multi-Fidelity Modeling of Laser-Driven Particle Acceleration." In the Proceedings of APS DPP 2023, Spokane, WA, December. LLNL-PRES-841185.

Mariscal, Derek A, and others. 2025. "Advancing IFE Science & Technology through Machine Learning and High-Repetition-Rate High-Energy-Density Experiments." In the Proceedings of IFE-STAR Conference, Breckenridge, CO, April. LLNL-POST-2011817.

Mariscal, Derek A, and others. 2025. "Autonomous Frameworks for HRR Laser-Plasma Diagnostics and Physics-Driven Control." In the Proceedings of LaserNetUS Users Meeting 2025, San Francisco, CA., July 2025. LLNL-PRES-872790.

Mariscal, Derek A, and others. 2025. "High Repetition Rate Experiments, Edge Technologies, and Real Time Processing." In the Proceedings of LaserNetUS Users Meeting 2025, San Francisco, CA., May 2025. LLNL-PRES-872790.

Zeraouli, Ghassan, and others. 2025. "Investigating Electron Heating and Transport through High Repetition Rate Experiments and Ensemble Modeling." In the Proceedings of LaserNetUS Users Meeting, Phoenix, AZ, July. LLNL-POST-2009515.

Matsubara, Hiroki, and others. 2025. "Investigation of Non-Thermal Electron Dynamics in Short-Pulse, Laser-Solid Interactions." In the Proceedings of LLNL Summer Scholar Poster Symposium, Livermore, CA, August. LLNL-POST-2009515.

23-ERD-037: Volumetric Additive Manufacturing of Gradient Composition Glass

Project Overview

Advanced optics, such as lasers or cameras, are currently limited by geometric or compositional restrictions on the silica glass components that act as focusing or refracting lenses. Currently, these glass components must be made of one homogenous material in a range of shapes and sizes limited by a few specialized vendors. However, additional flexibility and customization of these optical components could significantly improve the performance of these devices and expand the design space available to optics engineers, as would the capability to locally change the optical properties of these glass components by changing the composition of the glass as a function of location. To this end, we have developed a method to print and process gradient composition glass, using volumetric additive manufacturing (VAM) and direct ink writing (DIW), on-site at Lawrence Livermore National Lab.

Over the course of this project, we have explored methods to combine VAM and DIW, advanced our understanding and capabilities with glass VAM, and developed reliable methods to dope glass with different additives. We have developed and implemented a unique program to automatically generate DIW tool paths which result in specifically architected gradients by compensating for input/output lag in the ink composition and allowing the user to easily designate what gradient will be generated. As part of this project and others, a greyscale VAM projection technique was also developed to compensate for composition gradients in the VAM vial to ensure print fidelity. This project has also facilitated increasing the printable size and resolution of glass VAM from ~15 mm and 0.5 mm respectively to approximately 30 mm and 0.1 mm. A novel method of tiling VAM prints was also developed to compensate for the trade-off between resolution and size normally observed in VAM, producing a 30 mm long print with 0.1 mm features. Finally, we have fine-tuned methods to uniformly dope glass prints with metal ions to tailor aspects of the glass such as color, firing temperature, and refractive index, by soaking the unfired glass print in solutions of dissolved metal salts. This method also expands printable glass chemistries, as it does not require sourcing new nanoparticles for every glass composition.

Mission Impact

This exploratory research supports the ‘Accelerated Materials and Manufacturing’ and ‘Lasers and Optical Science and Technology’ Core Competencies. As a novel manufacturing capability, VAM permits 3D printing of many structures that are difficult or impossible to make even for other AM techniques, let alone conventional manufacturing. To highlight this capability, we successfully printed and characterized integrated double lens convex optics, double concave optics, and simple convex lenses which have focal points as small as 1 mm. New capabilities have also come from this project, such as the ability to print gyroscopic resonators which display a clear and intentional resonant frequency for use in navigation, as well as complex 3D microfluidic devices to control fluid flow. The team is currently in talks with both government and commercial entities to apply these capabilities.

Publications

De Beer, Martin, Galvan, Hazel R., Mittelberger, Daniel, Bhanvadia, Aftab, Lum, Jordan, Gothenquist, Sydney, Xia, Xiaoxing, Porcincula, Dominique, Walton, Beck L. 2025. "Tomographic volumetric additive manufacturing of centimeter-scale functional silica glass." Invited paper to *Advanced Materials Technologies*. LLNL-JRNL-2009155, in review.

Myers, Luke, Johanna Schwartz, Martin De Beer, Beck Walton, and Dominique Porcincula. 2024. "Development of transparent, particle-loaded photoresins for volumetric additive manufacturing of silica glass." *Journal of Polymer Science* 62, (January).<https://doi.org/10.1002/pol.20230654>. LLNL-JRNL-853706.

Posters

Gothenquist, Sydney, Luke Myers, Martin De Beer, Alyssa Troksa, Beck Walton, and Dominique Porcincula. 2024. "Digital Light Processing of Optical Quality Glass." (Poster Presentation at Gordon Research Conference on AM of Soft Materials, Smithfield, RI, August). LLNL-POST-863238.

Galvan, Hazel, Martin De Beer, Beck Walton, and Dominique Porcincula. 2024. "Recyclability of Glass Nanocomposite Resins Used in Computed Axial Lithography." (Poster Presentation at Gordon Research Conference on AM of Soft Materials, Smithfield, RI, August). LLNL-POST-868289.

De Beer, Martin, Hazel Galvan, Aftab Bhanvadia, Daniel Mittelberger, Beck Walton, and Dominique Porcincula. 2024. "Volumetric Additive Manufacturing of Transparent Silica Glass." (Poster Presentation at Gordon Research Conference on AM of Soft Materials, Smithfield, RI, August). LLNL-POST-1103617.

Presentations

Walton, Beck, Dominique Porcincula, Martin de Beer, Megan Ellis, Jungmin Ha, Luke Myers, Timothy Yee, Johanna Schwartz, Alyssa Troksa, Koroush Sasan, Nikola Dudukovic, Du Nguyen, and Rebecca Dyll-Spears, 2024, "Advancements in multimaterial glass Volumetric Additive Manufacturing (gVAM)." Presented at ACerS Glass and Optical Materials Division Meeting, Las Vegas, NV, May 2024.

Walton, Beck L., Dominique Porcincula, Martin de Beer, Megan Ellis, Jungmin Ha, Luke Myers, Timothy Yee, Johanna Schwartz, Alyssa Troksa, Koroush Sasan, Nikola Dudukovic, Du Nguyen, and Rebecca Dyll-Spears. 2023. "Towards robust UV-active 3D printing of glass: layer-based and layerless approaches." Presented at ACerS Glass and Optical Materials Division 2023 Meeting, New Orleans, Louisiana.

Porcincula, Dominique. 2023. "Volumetric Additive Manufacturing of Silica Glass." Presented at the Solid Freeform Fabrication Symposium, Austin, Texas.

Patents

Porcincula, Dominique, Beck Walton, Luke Myers, Martin De Beer, and Johanna Schwartz. 2024. "Photopolymer Resin Formulation for Fabrication of Solid Silica Glass Structures with Feature Sizes Greater than 5 mm." Submitted.

Records of Invention

Porcincula, Dominique, Beck Walton, Luke Myers, Martin De Beer, and Johanna Schwartz. 2023. "Optimized photopolymer resin formulation for fabrication of solid silica glass structures with feature sizes greater than 5mm." IL-13899.

23-ERD-038: Improving Quantum-Gate Fidelity with Universal Differential Equations

Project Overview

Quantum computing holds great promise for solving complex problems, but current devices are limited by high error rates of fundamental logical operations. These errors stem from the difficulty in accurately modeling and controlling the behavior of quantum hardware, which is affected by factors such as environmental noise and hardware imperfections. This project aimed to address these limitations by developing a new approach that combines physics-based models with data-driven corrections, allowing for more accurate prediction and control of quantum devices.

To achieve this, we created a framework that incorporates experimental data directly into the mathematical equations describing quantum dynamics. By doing so, we were able to identify and account for previously unknown sources of error, leading to improved accuracy in modeling and controlling quantum dynamics. The project also developed new optimization techniques that use high-performance computing resources to accelerate the design of control pulses for multi-qubit gates. As a result, the research demonstrated significant improvements in both the reliability and efficiency of quantum computing operations, paving the way for more practical and scalable quantum technologies.

Mission Impact

This research strengthens Lawrence Livermore National Laboratory's capabilities in quantum science by providing advanced methods for modeling and controlling noisy quantum devices. The new tools and techniques developed here enable more accurate simulations and efficient gate design, supporting future research and collaborations. The results are directly relevant to the missions of DOE and the NNSA, where reliable quantum computing is expected to drive progress in areas such as materials science, nuclear physics, and national security. By addressing key barriers to practical quantum computing, this work positions LLNL to lead in the development and application of next-generation quantum technologies, while also supporting broader federal initiatives in quantum information science.

Publications

Petersson, Anders, Stefanie Guenther, and Seung Whan Chung. 2025. "A time-parallel multiple-shooting method for large-scale quantum optimal control." *Journal of Computational Physics* 524, (March): 113712. <https://doi.org/10.1016/j.jcp.2024.113712>. LLNL-JRNL-866412.

Reddy, Sohail, Stefanie Guenther, and Yujin Cho. 2024. "Data-Driven Characterization of Latent Dynamics on Quantum Testbeds." *AVS Quantum Science* 6. LLNL-JRNL-858483.

Sentz, Peter, Stanley Nicholson, Yujin Cho, Sohail Reddy, Brendan Keith and Stefanie Guenther. 2025. "Learning thermodynamic master equations for open quantum systems." *Quantum* (under review). LLNL-JRNL-2005344

Posters

Sentz, Peter, Brendan Keith, and Stefanie Guenther. 2023. "Learning Thermodynamically Consistent Quantum Master Equations." (Poster Presentation at ICERM Workshop - Mathematical and Scientific Machine Learning, Brown University, June). LLNL-POST-850223.

Technical Reports

Sentz, Peter, Brendan Keith, and Stefanie Guenther. 2023. "Learning thermodynamic master equations for open quantum systems." LLNL. LLNL-SR-858172.

Keith, Brendan, Peter Sentz, Stanley Nicholson, and Stefanie Guenther. 2024. "Learning thermodynamic master equations for open quantum systems: Towards three-level systems and noisy data." LLNL. LLNL-SR-870963.

Presentations

Stefanie Guenther. "Gradient-based Optimization to Control Quantum Computing Testbeds." (Presented at Invited lecture at Brown University, Providence, November 2023).

Peter Sent, Brendan Keith, Stefanie Guenther. "Learning thermodynamically consistent master equations for open quantum systems." (Presented at ECCOMAS, Lisboa, Portugal, June 2024).

N. Anders Petersson. "Mitigating scaling barriers through time-parallel multiple shooting methods." (Presented at Quantum Optimal Control Workshop, Berlin, Germany, May 2024).

Stefanie Guenther. "Multi-qubit control using HPC resources." (Presented at IQUS Workshop - Pulses, Qudits and Quantum Simulations, Seattle, April 2024).

Stefanie Guenther. "Optimal Control for Quantum Computing via Time-Parallel Multiple-Shooting." (Presented at PinT Workshop, Brugge, Belgium, February 2024).

Anders Petersson. "Time-Parallel Control of Quantum Computing Devices." (Presented at Invited lecture at University New Mexico, Albuquerque, April 2024).

Anders Petersson. "Time-parallel multiple-shooting for multi-qubit optimal control." (Presented at IEEE Quantum Week, Quebec, Canada, September 2024).

Stefanie Guenther. "Optimal quantum control for multi-qubit operations via time-parallel multiple-shooting." (Presented at SIAM Conference on Computational Science and Engineering (CSE25), Fort Worth, Texas, U.S., March 2025).

Stefanie Guenther. "Optimal Quantum Control: Theory." (Presented at LLNL Quantum Summer School, LLNL, August 2023).

23-ERD-039: Water Security in a Snow-Free Future: The Science of Subsurface Water Storage

Project Overview

The impending loss of snowpack in the Western US requires new subsurface water storage solutions via 'managed aquifer recharge' (MAR) to achieve a resilient water supply. This research enhanced the applicability of state-of-the-art isotopic tracers and machine learning (ML) techniques to advance our understanding of the complex hydro-geological and ecosystem interactions that underly groundwater recharge processes. Our combined interpretation of isotopic water ages and sources in the context of land use shows that local infiltration of precipitation in open spaces is an important recharge mechanism, in addition to the managed arroyo recharge. Furthermore, trees utilize imported water in summer to meet evapotranspiration demand. Groundwater age prediction by ML relies on features related to (1) the source of groundwater recharge, (2) contaminant history, (3) aquifer materials, (4) well construction, and (5) geochemical reactions along flow paths. A machine learning pipeline to identify MAR locations in satellite images showed that engineered water management in MAR systems can disrupt or even reverse expected correlations between surface water dynamics and climatic variables. These findings provide physically interpretable insights into groundwater recharge and provide reproducible, interpretable, and transferable tools for data-driven MAR planning and groundwater sustainability under growing climatic and hydrological uncertainty.

Mission Impact

This LDRD enhanced our understanding of the Earth system through improved data gathering and assessments of mitigation strategies, thereby advancing the *Earth System Resilience* Mission Focus Area, as well as LLNL's *Earth and Energy Resilience* mission. The research strengthened the *Nuclear, Chemical, and Isotopic Science and Technology* Core Competency by developing quantitative interpretation methods for isotopic water age signatures. The ML objectives advanced the *High-Performance Computing, Simulation, and Data Science* Core Competency by developing new pipelines integrating satellite image analyses for real-world challenges with limited, noisy, heterogeneous, multimodal training data.

Publications

Lerback, Jory, Richard Bibby, Jacob Danielsen, Mike Garguilo, Emilio Grande, Jake Harm, Ken Minn, Jean Moran, Erik Oerter, and Ate Visser. 2025. "How Rains and Floods Become Groundwater: Understanding Recharge Pathways with Stable and Cosmogenic Isotopes." *Hydrological Processes*. <https://doi.org/10.1002/hyp.70020>. LLNL-JRNL-865947.

Azhar, Abdullah, Indrasis Chakraborty, Ate Visser, Yang Liu, Jory Lerback, and Erik Oerter. 2025. "Machine Learning Prediction of Tritium-Helium Groundwater Ages in the Central Valley, California, USA." *Water Resources Research*. <https://doi.org/10.1029/2024wr038031>. LLNL-JRNL-861411.

Posters

Dory, Chris, Ate Visser, Jory Lerback, Luis Sanchez-Valle, Eddie Ocampo, and Helen Dahlke. "Ag-MAR Suitability in the Tulare Lake Basin by Noble Gas and Stable Isotope Derived Parameters." Poster Presentation at Biennial Symposium on Managed Aquifer Recharge, Tucson, AZ, April 2024. LLNL-POST-862415.

Dory, Chris, Ate Visser, Jory Lerback, Luis Sanchez-Valle, Eddie Ocampo, and Helen Dahlke. "Ag-MAR Suitability in the Tulare Lake Basin by Noble Gas and Stable Isotope Derived Parameters." Poster Presentation at American Geophysical Union Fall Meeting 2023, San Francisco, December 2023. LLNL-POST-857872.

Lerback, Jory, Ate Visser, Erik Oerter, Richard Bibby, Jake Harm, Jean Moran, Emilio Grande, Jacob Danielsen, Ken Minn, and Mike Garguilo. "Utility of ^{35}S as a tracer for recent stormwater recharge to drought-stricken aquifers." Poster Presentation at American Geophysical Union Fall Meeting 2023, San Francisco, CA, December 2023. LLNL-POST-858103.

Lerback, Jory, Ate Visser, Alexander Jacob Harm, Richard Bibby, Emilio Grande, Jacob Danielsen, Ken Minn, Mike Garguilo, and Jean E. Moran. "Evaluating Underground Floodwater Storage Using Isotopes." Poster Presentation at Western Groundwater Congress, Lake Tahoe, CA, October 2024. LLNL-POST-870015.

Lerback, Jory, Erik Oerter, Ate Visser, Alexander Jacob Harm, Jacob Danielsen, Mike Garguilo, Ken Minn, Emilio Grande, and Jean E. Moran. "Stable oxygen isotopes constrain tree water demand and timing in an urban streamside ecosystem." Poster Presentation at American Geophysical Union Annual Meeting, Washington D.C., December 2024. LLNL-POST-871422.

Presentations

Jory Lerback, Ate Visser, Jake Harm, Jacob Danielsen, Mike Garguilo, Ken Minn, Emilio Grande, Erik Oerter, Richard Bibby, 2024, "Storm-chasing in aquifers." Presented at Biennial Symposium on Managed Aquifer Recharge, Tucson, AZ, April 2024.

Ate Visser, Tarun Allaparti, Abdullah Azhar, Indra Chakraborty, Alexander Jacob Harm, Jory Lerback, Yang Liu, Erik Oert, 2024, "Understanding Groundwater Recharge with Satellite Imagery, Machine Learning, and Isotopic Tracers." Presented at Western Groundwater Congress, Lake Tahoe, CA., January 2024.

Code

Chakraborty, Indra. 2024. *Ground Water Age Predictor (GWAP)*, v. 1.0.
<https://github.com/LLNL/GWAP>.

23-ERD-040: Pulsed-Plasma Deposition of Ultrathick Diamond-Like Carbon Films on Nonplanar Surfaces

Project Overview

Diamond-like carbon (DLC) is a hard-wearing material with broad commercial use as a protective and tribological coating in applications as diverse as tool bits, smart watches, and internal combustion engine piston heads. In addition, the low-Z carbon composition, robust mechanical properties, and amorphous microstructure are appealing characteristics for a next-generation ablator for inertial confinement fusion (ICF) and high energy density physics (HED) experiments. There are several central challenges to DLC fabrication that must be overcome for a material to be suitable in this role, among them the requirement for ultrathick (> 50 micron) coatings and deposition on nonplanar surfaces. It is therefore crucial to develop a control and understanding of film stress and of oblique angle deposition effects.

Pulsed-plasma magnetron deposition techniques were employed in this project with a combination of film characterization, Monte Carlo modeling of gas phase transport processes, and plasma diagnostics in order to investigate the interrelationship between process parameters, energetics of incident species, and resulting film properties. Films of high density (> 2.5 grams per cubic centimeter) were successfully deposited at conditions of high applied substrate bias (negative 50-100 V) with impurities of less than 5 at. % of Ar, O, and H. Deposition on rolling spherical substrates was demonstrated to thickness of <40 microns with tunable density in the range of 1.5-2.15 g/cm³.

Mission Impact

Two major platforms for ICF experiments are based on carbon: low-density, amorphous hydrocarbon glow discharge polymer, and high-density, crystalline diamond. This project provides a foundation for further development of a robust alternative ablator platform for ICF and HED experiments based on amorphous diamond-like carbon with tunable density and a scalable, robust fabrication method of physical vapor deposition (PVD). If realized, a new platform would open new opportunities in target design for these efforts. In addition to promoting avenues for program growth, the project supported a Core Competency of the Laboratory in Advanced Materials and Manufacturing and developed science and technology tools and capabilities relevant to meeting future national security challenges.

Publications, Presentations, and Patents

A. M. Engwall-Holmes et al., "High-Power Impulse Magnetron Sputter Deposition of Ultrathick Amorphous Carbon," *Fusion Science and Technology*, American Nuclear Society, April 8, 2025, 1–9, <https://doi.org/10.1080/15361055.2025.2502890>.

A. M. Engwall-Holmes et al., "Diamond-like carbon (DLC) coatings prepared by pulsed plasma physical vapor deposition." 25th Target Fabrication Specialists Meeting, San Diego, CA, August 25, 2024.

23-ERD-041: Breakthrough Performance with Context-Constrained Radiation Measurements

Project Overview

Traditional radiation detection approaches are limited by physical detector constraints and ambiguities in radiation signatures, often resulting in nuisance alarms and false negatives. This Context-Constrained Radiation Measurements (CCRM) project developed novel algorithms and system designs that leverage multimodal sensor data—such as LiDAR, cameras, magnetometers, geophones, and radiofrequency receivers—to constrain machine learning (ML) training data in real time, improving the sensitivity, accuracy, and reliability of threat detection. Key achievements include the development of explainable, context-aware ML methods, the creation and validation of extensive semisynthetic datasets, and the prototyping of new multimodal detector systems. The project has demonstrated order of magnitude reductions in nuisance alarms and improvements in threat source identification and characterization, positioning these advances for broad impact in nuclear nonproliferation and nuclear material security applications.

Our developed bonsai revalued random forest approach queries in real time on a completely unconstrained random forest model and can provide constrained estimates competitive to full retraining without large computational costs or computational time. In addition to the benefits to nuclear threat detection and characterization, this approach may have significant impact on other machine learning applications. For example, this technology can have significant impacts in data unlearning as related to removing invalid data (data poisoning) or removal of copywrote material (as is a concern in commercial applications).

Mission Impact

The CCRM project has delivered significant advances in multimodal radiation detection by integrating contextual sensor data and developing real-time, explainable ML algorithms. While the developments have been demonstrated for multimodal radiation detection applications that strengthen LLNL's nuclear nonproliferation mission, these same capabilities can be translated across multiple focus areas in the NNSA. For example, the context constrained approach can be used to enable a user to, in real time, identify what the optimal measurement configuration is for their detector based on the initial estimate of the measured material. This could improve efficiency of processes in materials diagnostics both for nuclear safeguards and for characterizing material used in the nuclear stockpile. Additionally, this bonsai approach to human-AI teaming allows analysts to constrain results in real time and identify what other contextual information would be most impactful in reducing uncertainties. This approach is sensor agnostic and could be used for many analyses leveraging feature-based machine learning architectures. The CCRM project further strengthens LLNL's position as the big AI lab and builds on the LLNL's science and technology investment strategy for Threat Preparedness and Response.

Publications

McFerran, Noah, Eric Albin, Bonnie Canion, Steven Czyz, Jonathan Dreyer, Owen Drury, Dhanush Hangal, Simon Labov, Karl Nelson, and Erik Swanberg. 2023. "Contextually aware roadside radiation measurement testbed." *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 1050, . LLNL-JRNL-843225.

Posters

Busching, Levi. 2025. "Real-time Object Bounding in LiDAR With Computer Vision." (Poster Presentation at LLNL Summer Student SLAM, Livermore, August). LLNL-POST-2010395.

Abstracts

McFerran, Noah. 2025. "Context Constrained Analysis of Radiation Measurements." Abstract. *2025 Symposium of Radiation Measurements and Applications*, LLNL-ABS-2003674.

Technical Reports

Hoang, Minh, and Noah McFerran. "Deep Learning and Vision-Language Models for Roadside Vehicle Classification and Characterization." 2024. LLNL-MI-858789.

Busching, Levi. "Real-time Object Bounding in LiDAR Data with Computer Vision." DOE Science Undergraduate Laboratory Internship. 2025. LLNL-TR-2010394.

Presentations

Noah McFerran, Bonnie Canion, Jonathan Dreyer, Dhanush Hangal, Ming Jiang, Irene Kim, Simon Labov, Brandon Morrison, Karl Nelson, Artur Dubrawski, Dan Howarth, Kyle Miller, Chi-En Teh, Minh Hoang, Curtis Chou, "Breakthrough Performance with Context Constrained Radiation Measurements, LLNL-PRES-864864." (Presented at LDRD Mid-Project Review, LLNL, May 2024).

Minh Hoang, Noah McFerran. "Deep Learning and Vision-Language Models for Roadside Vehicle Classification and Characterization, LLNL-PRES-858889." (Presented at LLNL SULI Student Presentation, LLNL, January 2024).

Noah McFerran, Simon Labov, Caleb Mattoon, Karl Nelson, Joseph O'Brien, Minh Pham, Lisa Her, Dan Howarth, Chi-En Teh, Artur Dubrawski. "Multimodal Measurement System. Part of LLNL-PRES-865661." (Presented at Sponsor Visit, LLNL, June 2024).

Noah McFerran, Bonnie Canion, Jonathan Dreyer, Dhanush Hangal, Ming Jiang, Irene Kim, Karl Nelson, Simon Labov. "Context Constrained Analysis of Radiation Measurements." (Presented at Symposium on Radiation Measurements and Applications, Berkeley, July 2025).

Curtis Chou. "Context to Context Constrained Analysis." (Presented at Science Undergraduate Laboratory Internship, Livermore, August 2023).

Noah McFerran. "Contextually Aware Roadside Radiation Detection Systems." (Presented at PLS Postdoctoral Researcher Seminar Series, Livermore, August 2023).

Bonnie Canion. "Multimodal Measurement System for Radioactive Material Detection." (Presented at 2025 Global Security External Review Committee Meeting, Livermore, May 2025).

Noah McFerran. "Multimodal Radiation Detection." (Presented at NSSC Summer School 2025, Livermore, June 2025).

Noah McFerran, Irene Kim. "Nuclear Threat Detection." (Presented at Global Security Road Show, Livermore, August 2023).

Noah McFerran. "Nuclear Threat Detection using Machine Learning." (Presented at Sponsor Visit, Livermore, August 2023).

23-ERD-042: High-Pressure-Temperature Phase Diagrams and Free Energies from First Principles

Project Overview

The motivation for this research was to improve our ability to predict material properties under conditions of high pressure and temperature, such as those encountered in planetary interiors or dynamic compression experiments. Accurately modeling how materials respond in these extreme environments is challenging, as their behavior is influenced by a complex interplay of atomic motion, entropy, and electronic effects. There is a need for computational approaches that can capture these factors with both accuracy and efficiency, enabling researchers to better interpret experimental results and guide the design of future experiments.

To address these needs, our team developed and tested new computational techniques that combine first-principles simulation methods with advanced machine learning capabilities. We designed a method for predicting the stability of material structures directly at finite temperatures, enabling more accurate phase diagram calculations. In addition, we introduced a more efficient approach for computing the entropy of liquids and liquid mixtures, which is crucial for understanding their behavior at high temperatures. We also developed machine learning force fields that incorporate corrections for temperature and electronic effects, further improving the accuracy of our simulations. Our results demonstrate that these new tools can deliver reliable predictions of phase stability and material properties with significantly greater efficiency than previous methods. This advancement will help guide and interpret high-pressure experiments, support scientific discovery, and strengthen national capabilities in high energy density science and materials research.

Mission Impact

This research directly strengthens Lawrence Livermore National Laboratory's (LLNL) core capabilities in high energy density science, advanced simulation, and data-driven materials modeling. By developing new methods for predicting material behavior at high pressures and temperatures, including machine learning tools that improve accuracy and efficiency, the project enables LLNL to better interpret results from dynamic compression experiments and to design materials for extreme environments. These capabilities are critical for supporting the Department of Energy and the National Nuclear Security Administration's missions related to stockpile stewardship, national security, and scientific discovery. The new computational tools and approaches also open avenues for future research, attract new scientific talent, and position LLNL to address emerging challenges in materials science, planetary physics, and other fields important to federal agencies.

Publications, Presentations, and Patents

Kwangnam Kim, Yaye Badjo, Arpit Agrawal, Cristine Wu, and Stanimir Bonev, 2025, "First principles study for melting curve of Sn at high pressures up to 185 GPa", *Physical Review B*, Submitted.

Amy Coleman, et al., 2025, "Body-centered cubic phase transformation in Au ramp compressed to TPa pressures," *Physical Review Letters*, Accepted.

Agrawal, Arpit, and Stanimir Bonev. "Exploring the Crystal-to-Amorphous Transition in NiTi Using Metadynamics." Poster Presentation at American Physical Society, March Meeting, Minneapolis, MN, March 2024. LLNL-POST-1092669.

Agrawal, Arpit, and Stanimir Bonev. 2024. "Predicting crystal structures at finite temperature from the liquid phase." (Poster Presentation at LLNL Postdoctoral Symposium, Livermore, LLNL, August). LLNL-POST-1104188.

Nguyen, Cong Kien, and Stanimir Bonev. "Temperature-dependent machine learning interatomic-potentials for metallic systems." Poster Presentation at LLNL Postdoctoral Symposium, Livermore, LLNL, August 2024. LLNL-POST- 1104273.

Arpit Agrawal, Stanimir Bonev. "Predicting Crystal Structures from Molten Phases at Extreme Pressures." Presented at American Physical Society, March Meeting, Minneapolis, MN, March 2024.

Kwangnam Kim, Stanimir Bonev. "Predicting entropy of liquids at extreme conditions by thermodynamic integrations with machine-learning force fields." (Presented at American Physical Society, March Meeting, Minneapolis, MN, March 2024.

Stanimir Bonev, Arpit Agrawal, "Predicting high-pressure phase diagrams starting from the liquid." Presented at The 61st European High Pressure Research Group conference, Thessaloniki, Greece, September 2024.

Stanimir Bonev, Arpit Agrawal, Rasool Ahmad. "Can we compute high-pressure melting curves without knowledge of the crystalline structure?." Presented at The 62nd European High Pressure Research Group, Manchester, U.K., September 2025.

Rasool Ahmad, Stanimir Bonev. "Exploring Compressed Lithium through machine learning learning-assisted metadynamics." Presented at APS 24th Biennial International Conference on the Science of Compression in Condensed Matter, Washington, D.C., June 2025.

Rasool Ahmad, Stanimir Bonev. "Exploring Compressed Lithium through machine learning learning-assisted metadynamics." Presented at American Physical Society March Meeting, Anaheim, CA, March 2025.

Kwangnam Kim, Stanimir Bonev. "Integrating thermodynamic integrations with machine-learning force fields for Predicting entropy of liquids at extreme conditions." Presented at APS 24th Biennial International Conference on the Science of Compression in Condensed Matter, Washington, D.C., June 2025.

Stanimir Bonev, Arpit Agrawal, Rasool Ahmad, Kwangnam Kim. "Predicting high-pressure phase diagrams starting from the liquid." Presented at Goldschmidt, Prague, Chechia, July 2025.

Kien Nguyen-Cong, Stanimir Bonev, 2025, "Temperature dependent interatomic machine-learning potentials of metallic systems." Presented at APS Global Summit 2025, Anaheim, CA, March 2025.

Kien Nguyen-Cong, Stanimir Bonev, 2025, "Temperature- and ab initio functional-dependent machine learning interatomic potentials for high-pressure materials." Presented at APS 24th Biennial International Conference on the Science of Compression in Condensed Matter, Washington D.C., June 2025.

23-ERD-043: Modular Autonomous Experimentation for Biological Applications

Project Overview

The Modular Autonomous Research System (MARS) was created to address a key challenge in scientific discovery: experiments are often slow, require significant manual labor, and generate data that is not easily integrated across different tools. This limits how quickly scientists can explore new materials, processes, and chemical reactions. Our motivation was to design a system that makes research faster, more reliable, and adaptable by combining automation with artificial intelligence. By doing so, we aimed to reduce human error, accelerate discovery, and allow researchers to quickly test many possibilities that would otherwise take months or years.

Our approach was to build a flexible platform that connects laboratory robots, measurement instruments, and a central data system, all guided by artificial intelligence. MARS integrates liquid handling robots, robotic arms, and plate readers with an intelligent decision-making system that chooses the most informative experiments to run next. This creates a closed loop where experiments are performed automatically, the data is analyzed in real time, and new conditions are immediately tested.

Through this work, we demonstrated that MARS can carry out multiple experiments with little or no human intervention, adapt to different scientific problems, and handle uncertain or noisy measurements in a robust way. The results show that modular and intelligent automation can significantly accelerate the pace of discovery, providing a model for future self-driving laboratories. This approach addresses the growing scientific need for adaptable, data-driven research platforms that can keep up with the complexity and scale of modern science.

Mission Impact

This research advances Lawrence Livermore National Laboratory's mission by creating new capabilities for autonomous experimentation that accelerate discovery in chemistry, materials science, and biotechnology. MARS provides a flexible platform for integrating robotics, instrumentation, and artificial intelligence in ways that can reduce development timelines, improve reproducibility, and enable rapid exploration of complex design spaces. These capabilities have direct impact on Department of Energy and National Nuclear Security Administration priorities, including the development of advanced materials, support for energy resilience, and maintaining leadership in autonomous experimentation systems. Beyond DOE/NNSA, the approach is relevant to other federal agencies such as the National Science Foundation and the National Institutes of Health, where adaptive, high-throughput experimentation can drive innovation in areas ranging from sustainable manufacturing to biomedical discovery. By establishing a robust, modular framework and demonstrating its utility on diverse problems, this work opens new research directions for LLNL programs and positions the Laboratory as a leader in the emerging field of self-driving laboratories.

Presentations

Oyarzun, Diego I., Aldair Gongora, Jesus Fuentes, Nimit Deshpande, and Erika Ramos. "MARS: Modular Autonomous Research System for accelerated discovery." Talk at the Scientific Discovery in the AI Age Conference, Argonne National Laboratory, Argonne, IL, April 2025.

23-ERD-044: High-Performance-Computing-Enabled Detection System for Petabyte-Scale Astronomy Surveys

Project Overview

Modern astronomical surveys collect enormous volumes of wide-field imaging data that contain far more information about the solar system than is extracted by standard detection pipelines. Many asteroids are either too faint to be detected in individual images or were serendipitously imaged years before their official discovery, leaving valuable information unused. This project was motivated by the need to fully exploit archival and ongoing survey data to improve asteroid discovery, orbital accuracy, and planetary defense readiness, especially in anticipation of next-generation facilities such as the Vera C. Rubin Observatory.

We developed new probabilistic, computational, and high-performance computing methods to detect and recover faint solar system objects across multi-year survey baselines. The project produced three tightly connected results. First, we built an automated prediscovery pipeline that searches archival survey images for earlier detections of newly discovered near-Earth asteroids, using full orbital uncertainty propagation and statistical linking to control false positives. Second, we developed a general theoretical framework that quantifies how detection sensitivity degrades when stacking images along imperfect trial orbits, enabling principled and efficient digital tracking searches across nonlinear orbital motion. Third, we implemented these ideas at scale using a specialized high-performance computing architecture that enables survey-wide, multi-year digital tracking searches over extremely large orbital parameter spaces.

Applied to data from the Zwicky Transient Facility, these methods successfully extended asteroid observational arcs by years, reduced orbital uncertainties by orders of magnitude, and demonstrated the feasibility of detecting objects far below single-exposure limits. Collectively, the results establish a scalable pathway for extracting substantially more scientific and planetary defense value from existing and future astronomical surveys.

Mission Impact

This research directly advances Lawrence Livermore National Laboratory missions in planetary defense, space situational awareness, and data-intensive science. The project delivers new end-to-end capabilities for discovering, recovering, and refining orbits of solar system objects using national-scale computing resources, positioning the Laboratory to play a leading role in exploiting Rubin Observatory, Near-Earth Object Surveyor, and future survey data. The work opens new research directions in probabilistic orbit determination, large-scale digital tracking, and survey analytics, while strengthening connections between astrophysics, applied mathematics, and high-performance computing. The results are highly relevant to Department of Energy and National Nuclear Security Administration interests in planetary defense, as well as to National Aeronautics and Space Administration and other federal agencies responsible for near-Earth object detection, impact risk assessment, and long-term monitoring. The project led to funded work from NASA for developing asteroid detection methods for the Roman Observatory. Furthermore, the methods developed have direct connections to space domain awareness with funded projects in the Global Security in the Space Science and Security Program.

23-ERD-047: Towards a More Predictive Framework for Laser-Driven Particle Sources through Experimental Data-Informed Machine-Learning Models

Project Overview

Laser-driven particle acceleration (LDPA) has emerged as a critical technology for high-energy-density physics applications since its discovery at Lawrence Livermore National Laboratory twenty years ago. However, realizing the full potential of these particle sources requires understanding the fundamental acceleration mechanisms and developing enhanced target designs for improved performance. This research addressed the need for controllable, high-performance laser-driven proton sources through two complementary approaches: experimentally investigating sheath field dynamics in multi-picosecond laser regimes and developing novel three-dimensional printed microstructured targets to achieve enhanced particle acceleration.

Our approach combined experimental measurements of accelerating fields using proton radiography techniques with systematic scaling studies of additively manufactured targets with controlled density gradients. The research achieved significant milestones including the first direct measurements of Target Normal Sheath Acceleration (TNSA) sheath fields in the multi-picosecond regime for pulse durations from 0.6 to 10 picoseconds, demonstration that longer pulse durations sustain stronger electric fields for extended periods enabling enhanced proton acceleration, and validation of microstructured targets achieving record proton energies of 105.5 MeV with conversion efficiencies up to 8 percent compared to ~1-2% percent for conventional targets. These results provide fundamental understanding of acceleration mechanisms in unexplored parameter regimes and demonstrate practical pathways to high-flux applications in fusion energy research, medical physics, and national security applications.

Mission Impact

This research directly supports LLNL missions in high-energy-density science, inertial confinement fusion, and advanced diagnostic capabilities. The experimental measurements of sheath field dynamics provide fundamental understanding needed to optimize laser-driven particle sources for proton radiography applications critical to stockpile stewardship missions, while enhanced target designs provide pathways to high-flux sources needed for proton fast ignition concepts in inertial fusion energy. The work establishes new experimental capabilities for measuring electromagnetic field evolution in laser-plasma interactions, advancing objectives in plasma physics and high-energy-density science. The research supports NNSA missions through improved diagnostic capabilities for high-energy-density experiments and provides foundational understanding for optimizing advanced high-intensity short-pulse laser systems including the National Ignition Facility Advanced Radiographic Capability. The demonstrated performance improvements in microstructured targets offer practical benefits for applications requiring high-energy, high-flux particle sources while reaffirming LLNL leadership in novel target design and additive manufacturing for laser-plasma applications.

Publications

Simpson, R.A., Mariscal, D.A., Kim, J., Lemos, N., Grace, E.S., Swanson, K.K., Scott, G.G., Djordjevic, B.Z., and Ma, T. "Investigation of boosted proton energies through proton radiography of target normal sheath acceleration fields in the multi-ps regime," *Physics of Plasmas* 30, 103103 (2023). <https://doi.org/10.1063/5.0157214>

Tochitsky, S.Ya., Lemos, N., Simpson, R.A., Grace, E.S., Pak, A., Ma, T., Luoma, J.J., Fiuza, F., Haberberger, D.J., Haid, A., Knolker, K., and Joshi, C. "High-energy ion beams generated with high efficiency using laser-driven 3D microstructures," (Accepted, 2025).

Presentations

Scaling laser-driven ion acceleration to the inertial fusion energy regime, HEDS-OPIC, 2025.

Scaling laser-driven ion acceleration to the inertial fusion energy regime, US-Japan Inertial Fusion Energy Workshop, 2024

Investigation of enhanced laser-driven proton acceleration for fast ignition inertial fusion energy experiments, High Impact Talk at HEDSA Meeting, 2024.

Investigation of enhanced laser-driven proton acceleration for fast ignition inertial fusion energy experiments, Seminar at the Fraunhofer Institute for Laser Technology, 2024.

NIF Discovery Science Platform Development - Exploration of 3D-Printed Microstructured Targets for an Enhanced Isochoric Heating Platform on the NIF-ARC Facility, NIF/JLF User Group Meeting, 2023.

Development of a TNSA proton radiography platform on the world's most energetic laser - The National Ignition Facility Advanced Radiographic Capability, Optica Imaging Congress, 2023.

Development of a short pulse neutron source using the NIF-ARC laser, LENS Workshop on Laser-Driven Neutron Sources, 2023.

Temporally-shaped ARC Short-pulses for Studying Time-dependent Laser-Driven Particle Acceleration, National Ignition Facility User Group Meeting, 2023.

Investigation of Boosted Proton Energies through Proton Radiography of Target Normal Sheath Acceleration Fields in the Multi-ps Regime, APS Division of Plasma Physics, 2022.

23-ERD-049: Materials for Energy Management across the Electromagnetic Spectrum

Project Overview

Electrification of the United States has been a major driver of economic growth, powering industrialization, modern manufacturing, and the digital economy. Today, further economic and environmental benefits can be realized by improving the energy efficiency of the technologies we have come to rely on. This project focused on enhancing the energy efficiency of two cornerstone technologies of modern society: electronic displays and building climatization. While these two technologies operate in different parts of the electromagnetic spectrum (the visible and infrared, respectively), they share a common potential technological solution: electrically-driven displays that change reflectivity. In this work, we developed the first multipixel multicolor reflective display that achieves multi-colorization with fast-changing structural color. In the course of this demonstration, we quantified the structural changes that occur across different time and length scales and resolved device sealing issues, enabling operation of these devices over months (as opposed to days previously). We furthermore developed two reflectivity changing devices in the infrared and demonstrated how these technologies can be used to reduce climatization demands for both smart window and smart wall technologies. Implementing such a device in a scaled down mock room resulted in 10 degree Celsius change.

Mission Impact

This work broadly developed science and technology tools and capabilities to meet future national security challenges. Approaches that enable greater energy efficiency without sacrificing the performance of existing higher power-consuming technologies are highly desired across many applications areas in the Department of Energy (DOE), defense, and industry. The DOE has been particularly interested in technologies that may reduce building heating/cooling demands, like smart windows. Similarly, more energy efficient displays and personal electronics have had a long and ongoing evolution, and reflective displays or “electronic paper” represent a step-change technology.

Presentations

A. Abelson *et al.* “Electrically-tunable intersubband plasmon absorption in carbon nanotube films.” 2024 Electrochemical Society Meeting. San Francisco, CA, May 27, 2024. MA2024-01 901

A.M. Hiszpanski *et al.* “Thermal management using carbon nanotube devices with dynamic reflectivity.” 2024 Materials Research Society Fall Meeting. Boston, MA, Dec. 3, 2024. NM01.03.07

A. Cardenas *et al.* “Improved lifetime of an electrophoretic display based on solvent and sealant engineering.” TMS 2024 Conference, Orlando, FL, March 5, 2024.

A. Troksa *et al.* “A Low-powered Fast-response Colored Electrophoretic Display Based on Structural Color.” TMS 2024 Conference, Orlando, FL, USA

A. Troksa *et al.* “Dynamic Interplay of Color Transitions and Particle Behavior in α -Fe₂O₃/SiO₂ Nanoparticle-Based Electrophoretic Displays. Electrophoretic Deposition VIII: Fundamentals and Applications.” October 12-16, 2025, Calabria, Italy.

Patents

A. Abelson, A.M. Hiszpanski, S.J. Park, P.M. Jean-Remy, E.R. Meshot, S.F. Buchsbaum, T. Nakotte. “Products made with vertically aligned carbon nanotubes for modulating transmission of light.” 2025, Patent Application No.: 63/651601

24-ERD-034: Laser Architecture Scaling for Efficient Inertial-Fusion-Energy Drivers

Project Overview

LLNL's demonstration of a self-sustained, burning deuterium-tritium plasma in August 2021 and multiple successful demonstrations of fusion ignition since December 2022 sparked renewed interest and investment into the development of future fusion pilot plants based on inertial fusion energy (IFE). Recently, the DOE Fusion Energy Sciences program sponsored a "Basic Research Needs" (BRN) workshop to determine the technology readiness levels of several critical aspects of IFE development. In the final BRN report, the status of laser-based driver technology was rated at "low fidelity," due to the uncharted territory of delivering high pulse energies (~10kJ/beamline) at high repetition rates (10Hz) and efficiencies (>10%). To achieve the laser performance required for IFE power plants, multiple key technical challenges must be addressed: 1) aperture scaling of efficient laser materials, 2) optical damage constraints, 3) pump system costs, 4) large beamline footprint, and 5) power/thermal effects handling. With recent advances in laser technology and the current global excitement around IFE, a renewed exploratory research study on high power, efficient beamline concepts is timely and can support multiple future laser programs aimed at both energy security and national security applications.

In this LDRD project, an exploratory research study was conducted into higher risk, yet potentially transformational laser technologies to address multiple challenges of future inertial fusion energy beamlines. Through a combination of laser physics modeling efforts, proof-of-principle experimental demonstrations, and detailed technical discussions with subject matter experts, innovative concepts aimed at advancing laser performance to IFE-relevant levels were developed or identified. These concepts include beamline architecture configurations that allow the use of smaller, more efficient laser materials, as well as high power diode pumping designs, optical coatings for high fluence operation, a scalable concept to mitigate thermal-stress-induced depolarization losses, and more. Additionally, this LDRD connected two of LLNL's complex laser physics modeling tools through a feedback loop to support future rapid design optimization. The upgraded modeling capabilities and advanced concepts were combined to generate multiple high-level beamline design examples and compare performance expectations using various laser materials. These results lay the groundwork for the next phase of research under an upcoming LDRD, which will conduct a systems architecture design study and experimentally validate key technologies in support of LLNL fusion missions.

Mission Impact

This exploratory research (ER) LDRD advanced laser technology and developed science and technology tools and capabilities to meet future national security and energy security challenges. The results of this work could enable laser performance scaling to IFE beamline levels, and are applicable to current and future energetic laser systems suited for various LLNL/NNSA missions, including a wide range of HED experiments. In doing so, this LDRD supported the Investment Strategy's 3-5 Year Vision for both the Lasers and Optical Science and Technology and High Energy Density Science Core Competencies. This LDRD also directly supported LLNL's Inertial Fusion Energy Initiative, attracted industry partners and collaborators for future programs, and

continued LLNL's and the U.S.'s leadership within the worldwide lasers and fusion communities. Finally, the upgraded modeling capabilities and advanced concepts explored within this LDRD supported multiple successful internal and external funding proposals, including a direct expansion of this ER into a Strategic Initiative, involving large teams from multiple directorates as well as industry partners.

Publications

Crump, Paul, and William Fenwick. 2025. "Performance scaling of high-power diode laser pumps for fusion applications." In the Proceedings of SPIE Photonics West, San Francisco, California, USA, January. <https://doi.org/10.1117/12.3042712>. LLNL-CONF-872145.

Batysta, Frantisek, Anthony Vella, Saumyabrata Banerjee, Issa Tamer, Drew Willard, Emily Sistrunk, Brendan Reagan, and Thomas Spinka. 2025. "Depolarization self-compensation in high-power lasers enabled by a mid-cavity quartz rotator." *Optics Express*. Accepted Manuscript. LLNL-JRNL-2008727.

Crump, Paul, William Fenwick, Mohamed Elattar, Issa Tamer, Karl Haeusler, Mackenzie Nelson, Jos Boschker, Andrea Knigge, and Robert Deri. 2025. "Diode Laser Pumps for Future Inertial Fusion Energy Systems: Status and Perspectives." *Optics Express*. Accepted Manuscript. LLNL-JRNL-2008670.

Banerjee, Saumyabrata, Frantisek Batysta, Issa Tamer, Thomas Galvin, Robert Deri, Taylor Olsen, William Mixer, Justin Galbraith, Sandrine Herriot, Samuel McLaren, Leily Kiani, Elizabeth Grace, Zbynek Hubka, Emily Sistrunk, Thomas Spinka, and James McCarrick. 2025. "Stacked-Mosaic Amplifier and Diode Delivery Concept for kJ-class Inertial Fusion Energy Laser Driver." *Optics Express*. Accepted Manuscript. LLNL-JRNL-2009240.

Abstracts

Tamer, Issa, Robert Deri, Saumyabrata Banerjee, Frantisek Batysta, Justin Galbraith, Thomas Galvin, Elizabeth Grace, Zbynek Hubka, Leily Kiani, Emily Sistrunk, Samuel McLaren, Brendan Reagan, Thomas Spinka, and Tammy Ma. 2024. "Development of Multi-kJ, Efficient Lasers for Inertial Fusion Energy." Abstract. *10th International Conference on Ultrahigh Intensity Lasers (ICUIL)*, LLNL-ABS-863536.

Tamer, Issa, Robert Deri, Saumyabrata Banerjee, Frantisek Batysta, William Fenwick, Justin Galbraith, Thomas Galvin, Elizabeth Grace, Zbynek Hubka, Leily Kiani, Emily Sistrunk, Samuel McLaren, Brendan Reagan, Thomas Spinka, and Tammy Ma. 2024. "Diode-Pumped Solid State Laser Development for IFE: Progress and Technology Requirements." Abstract. *IEEE Photonics Conference (IPC)*, LLNL-ABS-864658.

Presentations

Issa Tamer, Robert Deri, Saumyabrata Banerjee, Frantisek Batysta, William Fenwick, Justin Galbraith, Elizabeth Grace, Sandrine Herriot, Zbynek Hubka, Leily Kiani, Emily Sistrunk, Samuel McLaren, William Mixter, Taylor Olsen, Brendan Reagan, Thomas Spinka, Tammy Ma, 2024, "Development of Multi-kJ, Efficient Lasers for Inertial Fusion Energy." (Presented at 10th International Conference on Ultrahigh Intensity Lasers (ICUIL), Cozumel, Mexico, September 2024).

Issa Tamer, Thomas Galvin, Samuel McLaren, 2024, "Modeling IFE Laser Beamlines at LLNL." (Presented at VBL++ User's Workshop, University of California Livermore Collaboration Center (UCLCC), Livermore, CA, June 2024).

Issa Tamer, Robert Deri, Saumyabrata Banerjee, Frantisek Batysta, William Fenwick, Justin Galbraith, Thomas Galvin, Elizabeth Grace, Zbynek Hubka, Leily Kiani, Emily Sistrunk, Samuel McLaren, Brendan Reagan, Thomas Spinka, Tammy Ma, 2024, "Diode-Pumped Solid State Laser Development for IFE: Progress and Technology Requirements." (Presented at IEEE Photonics Conference, Rome, Italy, November 2024).

Issa Tamer, 2025, "DPSSL Beamline Demonstrator Performance Targets." (Presented at HEC-DPSSL Workshop 2025, Livermore, California, USA, March 2025).

William Fenwick, Robert Deri, Issa Tamer, 2025, "High Power Diode Requirements for Inertial Fusion Energy (IFE)." (Presented at HEC-DPSSL Workshop 2025, Livermore, California, USA, March 2025).

Issa Tamer, Saumyabrata Banerjee, Frantisek Batysta, Robert Deri, Eyal Feigenbaum, William Fenwick, Justin Galbraith, Thomas Galvin, John Heebner, Sandrine Herriot, Leily Kiani, Samuel McLaren, William Mixter, Taylor Olsen, Nathan Ray, Samuel Schrauth, Thomas Spinka, Katherine Velas, Anthony Vella, 2025, "Lasers for Next-Generation Fusion Facilities." (Presented at LLNL Board of Governors S&T Committee Meeting, Livermore, California, USA, March 2025).

Patents

Batysta, Frantisek, Anthony Vella, Saumyabrata Banerjee, Emily Link, Issa Tamer, and Brendan Reagan. 2025. "Compensation of Thermally Induced Depolarization in Laser Amplifiers." Submitted. US Patent Application 63/855,201 Filed on July 31, 2025

Batysta, Frantisek, Saumyabrata Banerjee, Issa Tamer, Thomas Galvin, and Robert Deri. 2025. "Stacked-Mosaic Amplifier and Diode Delivery for Inertial Fusion Energy Drivers." Submitted. US Patent Application 63/853,369 Filed on July 29, 2025

Records of Invention

Batysta, Frantisek, Saumyabrata Banerjee, Issa Tamer, Thomas Galvin, and Robert Deri. 2024. "Multi-Mosaic Amplifier and Diode Delivery Concept for High Energy, High Repetition Rate Laser for Inertial Fusion Energy (IFE) Driver." 2025-002.

Batysta, Frantisek, Saumyabrata Banerjee, Anthony Vella, Emily Link, Issa Tamer, and Brendan Reagan. 2024. "Quartz Rotator in the Reverser for Polarization Self-Compensation in Relay-Imaged Multi-Pass High-Average-Power Laser Amplifiers." 2025-198.

24-ERD-059: Addressing Fluidic Constraints on Interleaved Immersion Cooled High Brightness Laser Diodes for Next Generation Laser Systems

Project Overview

High-brightness, semiconductor laser diodes are critical components of next-generation laser systems for fundamental science, industrial, and national security applications. To meet the demand for higher brightness and more powerful lasers, improved thermal management of laser diode bar stacks is required. This work advances an immersion-cooled architecture for high-brightness laser diodes, where microchannel coolers circulate dielectric fluid directly across the bars to remove heat more efficiently than traditional backplane cooling. Advancement of this architecture was achieved by integrating fast-axis collimator (FAC) lenses into the system, as these lenses are essential for beam collimation but must be positioned very close to the diode facets. While immersion cooling has already demonstrated improved thermal performance, a concern remains that FAC lenses may obstruct fluid access to the microchannels and disrupt cooling. To address this, a modified cooler geometry was modeled using computational fluid dynamics (CFD), fabricated, and experimentally tested to increase inlet flow area and maintain effective cooling with lenses in place.

Experiments showed that FAC lenses had little impact on thermal resistance or temperature uniformity, while the modified cooler design reduced centroid wavelength spread, indicating improved flow distribution across the bar. Brightness—calculated as optical power divided by emitting area—was compared against a conventional baseline of 1 kilowatt per square centimeter from backplane-cooled laser diodes. Using immersion cooling, this project achieved 3.25 kilowatts per square centimeter without lensing (more than $3\times$ the baseline) and over $2\times$ the baseline with lensing. Brightness levels were ultimately limited by system pressure drop constraints rather than the cooling architecture itself. These findings show that FAC lenses can be successfully integrated with advanced cooling strategies to enable brighter, more efficient, and more reliable next-generation laser systems.

Mission Impact

This work directly supports the Lasers and Optical Science core competency. Reliable high-power laser diodes are of cross-cutting importance for LLNL programs requiring next-generation laser systems. The project has advanced the underlying science and engineering needed to progress record-breaking brighter laser diode packaging to meet programmatic demands. Establishing brighter laser diode bar stacks will allow laser scientists and engineers to design and build systems with better performance, lower cost, and improved SWaP (size, weight, and power). Continued LLNL investment in this area will help maintain institutional leadership and competitiveness in the development of laser systems for scientific, industrial, and national security applications.

Presentations

Cassada, Nicole, Devin Funaro, Matt Boisselle, Jack Kotovsky, and Kathy Jackson. "Immersion-cooled, High-brightness Laser Diode Stacks with Lensing for Next Generation Laser Systems." Presentation at the 25th Annual Directed Energy Science & Technology Symposium, April 2025.

25-ERD-011: Meeting Demand for Enriched Isotopes: Designing the Next Generation of Atomic Vapor Laser Isotope Separation

Project Overview

Domestic production of enriched isotopes is essential for U.S. national security, energy independence, and medical applications, but many key isotopes cannot be produced at scale using existing methods. This project advanced Atomic Vapor Laser Isotope Separation (AVLIS) by combining LLNL's strengths in atomic physics, laser engineering, and materials science.

The team discovered new laser-driven ionization pathways for gadolinium, achieving a sevenfold enrichment of Gd-152 and a twofold enrichment of Gd-160, and demonstrated that modern Titanium Sapphire lasers can enable selective isotope separation for certain elements.

Innovative laser techniques were developed. The team also built tunable, narrow-linewidth pulsed lasers spanning 570–680 nm using optical parametric methods, greatly improving spectroscopic capabilities. The team demonstrated the first application of narrow linewidth, nanosecond pulsed fiber lasers, which will enable the construction of higher energy per pulse fiber lasers. Enabling this scalable cost-effective technology to achieve high pulse energy operation without damage will expand this laser technology's application to AVLIS.

Materials modeling using density functional theory (DFT) provided new tools which will give insights into uranium diffusion and permeation in refractory metals and their compounds, helping to identify optimal coatings for AVLIS system components. These integrated advances enhance LLNL's technical capabilities and lay the groundwork for future domestic isotope enrichment.

Mission Impact

This research supports NNSA, DOE, and LLNL missions by enabling more efficient, scalable, and cost-effective isotope production, directly benefiting national security, advanced energy systems, and medical diagnostics. The project's advances in laser and materials technology strengthen LLNL's Core Competencies in nuclear and isotopic science, while rapid spectroscopic methods reduce analytical timelines and sample consumption for isotope separation. The development of new ionization pathways and robust components positions LLNL to address future challenges in isotope enrichment, including those needed for advanced nuclear fuel cycles and other needed isotopes.

Publications

Lauriola D., Savina, M., Raiwa, M., Harmon, W., Isselhardt, B. (2025). "Development and investigation of efficient resonance ionization mass spectrometry schemes of gadolinium," *Journal of Analytical Atomic Spectrometry*, LLNL-JRNL-2007314.

DOI <https://doi.org/10.1039/D5JA00325C>

25-ERD-048: Toward a High-Power Terahertz Vacuum Electronic Device

Project Overview

This LDRD studied a vacuum electronic device (VED) that produces high power and extremely high frequency radiation in G-band, by utilizing a Backward Wave Oscillator (BWO) based on WR3 standard waveguide, to be used as a source for Doppler velocimetry. This device is compact, fundamentally simple, and can be a useful source of sub-terahertz frequency radiation. This effort involved analytical calculations of the dispersion relation of the optimized slow wave structure (SWS), SUPERFISH calculations of the dispersion relation, COMSOL finite element simulations of the dispersion relation, and ICEPIC particle-in-cell (PIC) simulations of the SWS driven by an electron beam. The dispersion relation from the analytical derivation, SUPERFISH calculations, and COMSOL simulations were in excellent agreement. The ICEPIC PIC simulations demonstrated an output power of over 100 W, which exceeds the output power of about 1 W, demonstrated in an earlier design that our work was based on. Furthermore, whereas the earlier structure was designed using nonstandard waveguide, our design is integrated with standard WR3 waveguide.

A prototype SWS was fabricated using the DARPA-sponsored Digitized (LAM3D) technique by the innovator and collaborator Elve, Inc. The device was connected to a Vector Network Analyzer (VNA) setup using VDI VNA extender modules. The two port measurements performed on the fabricated devices resulted in good agreement with the dispersion relation that was calculated analytically, using SUPERFISH, and using COMSOL. This gives a great deal of confidence in the design that is predicted to output 100 W in ICEPIC PIC simulations.

Mission Impact

This project aligns with the Diagnostic Development Program in Weapons Physics and Design at LLNL, and therefore supports Stockpile and Enterprise Transformation. Another applicable Mission Focus Area is Integrated Deterrence and Technology Competition, as we will be able to analyze adversary capabilities as they aggressively pursue THz technologies and diagnostics. The primary mission space impacted would be for high spatial resolution Doppler velocimetry. Once demonstrated, this compact, high-power sub-THz source will be integrated into an optimized, high-precision Terahertz Doppler Velocimetry (TDV) system — a transformative diagnostic tool for real-time, non-invasive measurement of transient high explosive (HE) processes in extreme environments.

Publications

A.D. Andreev, A. Glick, E. Schamiloglu, N.B. Kostinski, and B.R. Poole, “Dispersion Model of a Rectangular, Sinusoidally Corrugated, 220 GHz Backward-Wave Oscillator (BWO),” *Proc. IVEC* 2024 (Monterey, CA, April 22-26, 2024), paper 12.1.

24-FS-012: Nondestructive Diagnostics of Laser-Conditioning Effectiveness of Deuterated Potassium Dihydrogen Phosphate

Project Overview

Potassium Dihydrogen Phosphate (DKP) and its deuterated analog, Deuterated Potassium Dihydrogen Phosphate (DKDP) are currently the material of choice for frequency conversion in mega-joule class laser systems. This is due to the current capability to grow large crystals with relatively high ultraviolet (UV) laser damage resistance. However, these crystals, when exposed to high fluence laser exposures from high-energy laser systems such as the National Ignition Facility (NIF), initiate bulk-damage, which can cause significant deterioration of the laser performance. Laser-conditioning (pre-exposing to gradually increasing laser fluence) these crystals, especially to short pulse length (500 ps) non-damaging laser pulses has been shown to be very effective at improving the bulk-damage resistance of DKDP. Even so, due to the variability from one crystal boule to another, the bulk laser-induced damage resistance of DKDP remains one of the key limiting factors in high-energy laser systems. As the NIF continues to increase the total amount of energy delivered to target and future mega-joule class laser systems are considered, additional improvements in the bulk-damage resistance of DKDP is required.

This feasibility study (FS) considered a supplementary laser-conditioning process to further increase the bulk-damage resistance of DKDP. Two DKDP crystal samples were purchased to help determine the magnitude and variance in the effect. One crystal was pristine and an effectiveness study of the supplementary laser-conditioning was performed by varying several process parameters (see publication in next section). The second test part was cut from a crystal previously used on the NIF, and served as a good proxy for the expected limit of this supplementary laser-conditioning process. Laser-induced damage tests were performed and compared on both crystal parts in regions that were laser-conditioned or laser-conditioned + supplementary laser-conditioning and both parts showed a significant increase in bulk-damage resistance where the supplementary conditioning process had occurred. This conclusively demonstrated that the supplementary laser-conditioning process was effective at increasing the bulk-damage resistance of DKDP crystals by $\approx 30\%$.

Mission Impact

This work strongly aligns with LLNL's core competency in Laser and Optical Sciences and Technology. The effort has demonstrated the feasibility of improved laser-conditioning methods, which enables enhanced energetics, performance, and stability of high-energy laser systems (e.g. NIF). Additionally, this reduces the risk when growing large DKDP crystals as the supplementary laser-conditioning process enables increased bulk-damage resistance. This enables the use of many crystal boules not currently viable for projects under consideration such as the Enhanced Yield Capability (EYC) for NIF which will help maintain and enhance the safety, security, and effectiveness of the U.S. nuclear weapons stockpile.

24-FS-030: Calculation of Phase Diagrams Optimized Materials with Passivating Oxides for Ultrahigh Temperature Ceramics Next Generation Delivery Systems

Project Description

Next generation extreme environment applications will be subjected to aerothermal conditions that will require the formulation of new materials that can maintain structural and mechanical integrity through the complex chemistries, temperatures, and mechanical stresses. Ultra-High Temperature Ceramics (UHTCs) are an attractive class of materials for this application due to their high temperature properties which can be exploited and tuned through the design of composites for a variety of high temperature applications. However, to efficiently explore the large phase space available for these novel composites, computational predictions must be utilized. This feasibility study explored the uncertainty associated with CALculation of PHase Diagrams (CALPHAD) predictions within the $Ti_{1-x}Zr_xB_2$ phase space using a combination of computationally derived inputs from Density Functional Theory (DFT) and experimentally derived inputs. A distribution of experimental inputs were explored with the goal of ultimately prioritizing and placing bounds on the number and types of necessary experiments for accurate phase predictions. The feasibility of this computationally validated experimental approach was proven, resulting in a streamlined experimental pathway for thermodynamic data collection targeted for CALPHAD.

This research built the foundation for pairing experiments on ceramics and the computational tool CALPHAD ultimately proving the feasibility of the approach. We successfully demonstrated that we are able to predict relative information gain in a CALPHAD model for an experiment, perform the experiment, and realize those model-information gains by performing a Bayesian update of our model parameters with ESPEI. Sample preparation pathways were developed for thermodynamic property measurements that can be used to extract the fundamental parameters needed as inputs for CALPHAD. The metric used to determine the uncertainty in CALPHAD was found to be a more universal method which can be used to drive computational directed experiments. This in turn will reduce the number of necessary experiments for an accurate prediction. Overall, this feasibility study built the foundation for a strong start on a larger scale study on ultra-high temperature ceramics.

Mission Impact

This feasibility study explored a simple pseudo-binary phase space using both experiments and the computational tool CALPHAD to build the foundation for understanding and quantifying the uncertainty in these computational predictions. The foundational understanding of how to quantify the uncertainty in CALPHAD predictions will enable the project team to create new ways of responding to national security challenges based on ceramic systems. These predictive and exploratory capabilities will be used to build into a larger scale project with a direct impact to National Security interests.

24-FS-031: Extending the Reach of Superconducting-Nanowire Single-Photon Detectors

Project Overview

There is accumulating evidence that non-equilibrium thermodynamic processes—such as the accumulation and delayed avalanche-like releases of energy in materials and devices—are limiting the sensitivity of detectors used in coherent neutrino scattering experiments, dark matter particle searches, axion searches, and superconducting (low-temperature solid-state) detectors. These material-dependent processes are underexplored and lack quantitative models. For ongoing axion searches (e.g., project BREAD), there is a need for low-background IR photon detectors sensitive to low-energy photons—up to 100 μm wavelength (down to 1 meV energy). This presents two competing requirements.

We proposed enhancing the photon energy sensitivity of the Superconducting Nanowire Single Photon Detector (SNSPD), currently the fastest, most sensitive, and lowest-noise superconducting photon counter. Achieving this requires a deeper understanding of the specific mechanisms of sensing and noise/background production, aligning with the broader goal of advancing knowledge of non-equilibrium processes.

Our approach combines experimental work and analysis of published data. It is widely accepted that a primary photon generates quasiparticles in a superconducting nanowire by breaking Cooper pairs. Thus, increasing energy sensitivity requires lowering the energy needed for quasiparticle production, which implies using materials with lower transition temperatures. In 2024, two groups at JPL demonstrated detection of 29 μm photons (using SNSPDs with type II superconducting nanowires) and 25 μm photons (using kinetic inductance detectors, where the primary photon breaks Cooper pairs in Al, a type I superconductor).

Much faster recovery time of the SNSPD compared to MKIDs after photon detection suggests that quasiparticle recombination is not the primary relaxation mechanism. This implies that detection may involve vortex liberation from pinning centers in type II superconducting nanowires, followed by vortex avalanches without significant quasiparticle production. If this mechanism is confirmed, it offers a path to developing detectors with both low background noise and low photon energy thresholds.

Dark counts/background events are believed to be caused by hot phonons originating from relaxation processes in the material. Phonons are less effective at liberating vortices from pinning centers than IR photons. A vortex-sensing mechanism would not require low T_c nanowire materials, reducing background noise from thermally generated quasiparticles.

The experimental goal of this LDRD was to acquire SNSPD sample devices and operate them at much lower temperatures (< 10 mK) than they had been operated with before (usually around 250 mK) and attempt to extend their sensitivity to wavelengths up to 100 μm .

In summary, by studying non-equilibrium processes in SNSPDs (a promising technology), we are opening a new research area. This has implications for developing the most sensitive photon and

particle detectors, as well as advancing condensed matter physics, non-equilibrium quantum statistical mechanics, and quantum information science.

Mission Impact

Advancing the understanding of non-equilibrium processes and improving SNSPD performance strengthens LLNL's leadership in cutting-edge detector technologies and quantum materials research. The lack of development in non-equilibrium quantum statistical mechanics for modeling real material processes poses a significant scientific challenge. Addressing this gap is critical for maintaining global leadership in science and technology (S&T) and supporting multi-domain deterrence.

Our results directly support LLNL's Core Competencies in Nuclear, Chemical, and Isotopic S&T by enabling advancements in detectors for neutrino, dark matter, and axion search experiments. This work also contributes to the development of quantum materials and LLNL's expertise in Advanced Materials and Manufacturing. The broader implications extend to LLNL's Strategic Advantage Mission Focus Area and Bio-Resilience Mission Focus Area due to the diverse applications of SNSPDs, including:

1. LIDAR systems
2. Quantum communications
3. Long-range space communications
4. Biomedical research

These applications are also critical for NASA and future cooled space IR-microwave telescopes.

Publications, Presentations, Patents

Work was presented (online) at the collaboration meeting of the DRD5 (superconducting and quantum detector R&D collaboration). "Energy accumulation and release in materials and dark matter searches and decoherence of qubits." CERN, Geneva, Switzerland. February 18, 2025. LLNL-PRES-2002859.

25-FS-002: Enhancing Photogrammetry for Surface Characterization

Project Overview

Photogrammetry, the reconstruction of three-dimensional geometry and surface color from photos, is attractive for surface characterization because it relies on relatively simple equipment and can be deployed flexibly in both laboratory and field environments. However, accuracy often degrades due to suboptimal image acquisition conditions, reflections, limited depth of field, and the lack of automation. Many traditional metrology methods, such as X-ray computed tomography and coordinate measuring machines, are impractical for in situ scenarios, large objects, reflective materials, or cases requiring color analysis for chemical change detection. This feasibility study aimed to evaluate and enhance photogrammetry for crucial applications at LLNL by identifying drivers of reconstruction inaccuracy, optimizing image acquisition and processing, and establishing where enhanced photogrammetry could serve as a primary characterization tool.

Our approach combined stakeholder engagement, controlled experiments, and prototyping of improved workflows. We worked with partners in the Space Program within Global Security, wind tunnel research collaborators, and engineering teams using gloveboxes to capture geometry through glass. Technically, we developed an end-to-end workflow emphasizing robust image acquisition and advanced processing to increase spatial fidelity and reduce artifacts.

We validated the workflow in a mock glovebox setting to emulate challenging in situ conditions, iterating on illumination, polarization, lensing, and capture automation. The resulting prototypical workflow improved input image consistency, increased detail, and reduced reflection artifacts, which together enhanced downstream reconstruction quality. We also assessed operational limits and trade-offs between spatial resolution, field of view, acquisition time, and environmental constraints to guide practical deployment.

- Prototypical glovebox photogrammetry workflow: Demonstrated improved image consistency and reconstruction accuracy through focus stacking, cross-polarization, and controlled illumination inside a glovebox mockup. This supports in situ characterization where relocation is infeasible.
- Hyperspectral photogrammetry: Generated three-dimensional reconstructions enriched with spectral bands to enable color-based surface characterization that can inform chemical state changes or material differentiation.
- Alternative reconstruction exploration: Evaluated three-dimensional Gaussian Splatting for scenes with significant view-dependent effects, informing when to augment traditional photogrammetry with appearance-aware methods.
- Capture automation: Implemented semi-automated rotation stage acquisition and initiated fully automated capture with a robot arm to standardize viewpoint sampling, reduce human error, and pave the way for scalable, repeatable inspection workflows.

Mission Impact

Surface characterization is integral to multiple mission areas, including inspection of manufactured components, monitoring of hazardous materials, and rapid before-and-after comparisons. This

feasibility study enhances LLNL's capability by improving the robustness and accuracy of photogrammetry through better image acquisition, artifact reduction, spectral characterization, and automation. The outcomes increase the utility of photogrammetry as a primary tool where traditional metrology is impractical, support non-contact measurement in gloveboxes and other constrained environments, and enable more agile, repeatable inspection workflows that benefit programs requiring timely, in situ assessments. This project supports the High Performance Computing, Simulation, and Data Science and Advanced Materials and Manufacturing Core Competencies.

Publications, Presentations, and Patents

“Robotic Monitoring: Automated Multi-Modal Virtual Inspection” CASIS 2025, Livermore, CA.

25-FS-004: Development of High-Power Near One Terahertz Quantum Cascade Lasers

Project Overview

The goal of this project is to advance the development of compact, high-power laser sources operating near 1 terahertz (THz) for use in high explosives diagnostic applications such as THz velocimetry, offering unprecedented spatial resolution compared to microwave velocimetry. In the last decade, quantum cascade lasers (QCL) have become an established technology at frequencies between 3 to 5 THz. However, high power low-frequency THz QCLs that operate below 2 THz are currently unavailable. A next generation high-power THz source in the 1 to 3 THz range, could substantially advance THz spectroscopy for applications in drug detection, biomedical imaging, and security screening, as many substances of interest (e.g., illicit drugs, biologically relevant molecules, and energetic materials) exhibit characteristic absorption resonances below 2 THz. To enable higher performance QCLs in the 1 to 3 THz frequency range requires a comprehensive study on the design of the laser waveguide. In this feasibility study we conducted a thorough THz QCL waveguide design investigation to achieve high confinement factor (Γ) and low gain threshold (g_{th}) in low frequency 1 THz QCLs and to the best of our knowledge, such a study has not been published in literature to-date. We also built expertise in conducting nanofabrication and characterization of THz QCLs during the project work so we are prepared to fabricate and test the newly designed 1 THz QCL which is being grown at Sandia National Lab's Center for Integrated Nanotechnologies (CINT). The proposal to CINT is being reviewed to move forward.

Results of our efforts include a new hybrid THz QCL waveguide structure that combines features of the conventional Metal-Metal (MM) and Semi-Insulating Surface Plasmon (SISP) waveguide structures, with the 1 THz hybrid MM-SISP waveguide utilizing a 3 μm GaAs-based plasmon layer with a $5 \times 10^{18} \text{ cm}^{-3}$ carrier concentration, achieving a $30 \text{ cm}^{-1} g_{th}$ minimum and 0.988Γ — over 10 times lower g_{th} and two-times higher Γ than a conventional SISP design with a 500 nm plasmon layer, which will result in a higher power laser. We also established nanofabrication processes for THz QCLs and characterized semiconductor materials properties in the THz regime since they are challenging to find using terahertz time-domain spectroscopy (TDS) and conducted detailed electromagnetic modeling to refine our design. This work also funded one round of growth and fabrication at SRI International of a baseline QCL in the literature, which did not result in lasing due to surface roughness, but was nevertheless informative for the next iteration of fabrication we plan to do to achieve a smoother surface. It is likely with several more rounds of fabrication, a refinement of the chemical recipe can be achieved to produce viable lasers.

Mission Impact

This project directly supports Stockpile and Enterprise Transformation by advancing THz source technology essential for the development of new high-explosive (HE) diagnostics, like THz velocimetry. These diagnostics will enhance our understanding of HE behavior and reduce uncertainties in HE models, thereby strengthening LLNL's capabilities in critical mission areas. Moreover, DHS is interested in THz applications for fentanyl detection. Should these lasers reach

high output powers, LLNL can come together to deliver a fast fentanyl detection system using our developed THz sources.

Publications

Ramker, Adam, Kaleb McClenathan, Zane Shellenbarger, Brian Poole, Natalie Kostinski, and Fatima Toor. *2d Trapezoidal Waveguide Design for near One Terahertz Quantum Cascade Lasers*. *Optical Engineering + Applications*. Vol. 13129: SPIE, 2024. <https://doi.org/10.1117/12.3028979>.

Presentations

Ramker, Adam, Zane Shellenbarger, Brian Poole, Natalie Kostinski, and Fatima Toor. "Design and Characterization of a Terahertz Quantum Cascade Laser for Fentanyl Detection." 2025 University of Iowa College of Engineering Research Open House, Iowa City, IA, USA, 2025.

25-FS-007: Detection of Fissile Material in Space Through Primary Cosmic Ray Interactions

Project Overview

Experiments performed by an LLNL team at the White Mountain Research center discovered that primary cosmic ray interactions on high-Z material produced large bursts of correlated neutrons. In fissionable material, these neutrons will start fission chains enhancing the neutron signature with a characteristic time signature. This signature could be a unique method for discovering fissionable material in challenging environments.

We performed a Geant4 based simulation study to estimate the signals and primary backgrounds for cosmic ray interactions on fissionable material. We studied multiple methods of detection of these signals at a variety of length scales from the material. Our analysis determined that there are unique, measurable signatures present that warrant additional study.

Mission Impact

This research represents an entirely new method of detecting fissionable material in challenging environments. These results will be used to support an array of follow-up studies to refine the simulations and analyses of these signals. Additionally, future work will include development and characterization of detection systems for this unique concept. This study may very well form the foundation for a new research program at LLNL to meet the NNSA's mission.

25-FS-011: Switch and Stitch Similar Subgraph Synthesizer

Project Overview

Government institutions utilize software from a wide array of development sources, including those written by large software companies, government contractors, and open-source repositories. Avoiding installation of malicious software components is an important national security endeavor. Automated analysis of previously unseen software is an active research area, and there is much research in the design of systems that compare new software artifacts to a large set of previously seen software records organized by various behaviors they contain. One attractive approach is to turn each compiled software binary into a graph representation and apply a graph similarity model that scores pairs of binaries by their relative similarity. When a pair is deemed similar, it is useful to know why, in the sense of providing explanations to security analysts regarding which portions of the software they should look into further.

This project studied automated explanations of results from graph neural network (GNN) similarity models applied to control flow graphs (CFGs) derived from compiled binaries. The team designed a reinforcement learning (RL) algorithm that, given a graph pair, updated its *state* (subsets of explanatory vertices), via *actions* (augmenting the explanatory vertices), and assigning *rewards* by checking the average degradation of similarity when subsets of the state are perturbed via structural swaps within the graph pair. The approach was evaluated using binaries compiled from source code obtained from Codeforces (a large, open, coding contest website), where the binaries are labelled in thousands of behavior categories, which is highly useful for training behavioral similarity models. The project determined that the basic approach was able to reveal small explanatory sets of vertices for many given similar pairs in minutes (per pair) on NVIDIA A100 GPU compute resources.

Mission Impact

Software assurance at DOE, other government agencies, and energy/telecom industries is a fundamental national security issue of high interest to Z-, E-, and N-programs. Automating the arduous tasks of understanding why approaches flag certain software components as having certain unexpected behaviors would save cyber security professionals countless hours of tedious and highly-skilled reverse engineering effort. This project performed fundamental research into one approach that could be operationalized for this purpose, if further hardened. More broadly, many LLNL missions involve complex data representations for which foundational models, such as large language models (LLMs) pretrained on volumes of text, are not directly applicable. This project made advancements in techniques for one specific mission-relevant data class (software binary representations), but the GNN- and RL-based approach could be used on many more tasks involving metadata-rich graph data, including analyses of social networks, chemical compounds, or cyber/physical systems.

25-FS-017: Quantitative Measurements of Dislocations in Metals for Advancing Predictive Simulations

Project Overview

LLNL applications require scientists to predict how materials evolve under various thermomechanical conditions. While this is achieved through physics-based simulations, uncertainty in the predictions of mechanical properties remains a serious challenge that limits the predictive capabilities of models because we lack methods to compare predictions of atomic-scale defects (dislocations) with experimental measurements. High energy X-ray diffraction (HEXRD) is the most relevant technique that can provide the necessary statistical information on dislocations. However, this technique is not yet quantitative because we lack a precise understanding of the relationship between X-ray diffraction patterns and the underlying material dislocation content and arrangements. To address this need, we used our novel computational X-ray diffraction method to simulate the effect of dislocations on the diffraction patterns. We compared virtual and experimental diffraction patterns. Results allowed us to clearly establish the relationship between X-ray diffraction patterns and the underlying dislocation structures, proving that it is feasible to quantitatively measure dislocation statistics with HEXRD. This project delivered a method that can provide the missing piece to LLNL's mechanical property simulations in advanced metals by obtaining experimentally long-needed quantitative dislocation data, which could fully enable predictive capabilities.

Mission Impact

This project's results are directly related to SD and PLS under the focus areas "Stockpile and Enterprise Transformation" and "Integrated Deterrence and Technology Competition". The HEXRD simulator can capture essential materials information from experiments already conducted on stockpile materials (surrogate and real) and allow us to design better experimental conditions for future testing. In addition, this same capability is directly relevant to the "Advanced Materials and Manufacturing" core as it can be used to finally understand the novel deformation mechanisms occurring in additively manufactured metals where dislocation configurations are unique.

25-FS-024: Intelligent Transformations for Differential Equations

Project Overview

Mathematical models in the form of differential equations are ubiquitous across scientific applications, including fusion, material science, and power grids. In many cases, applying a change of variables can simplify dynamics and improve solver performance. For example, transforming orbital dynamics into action-angle coordinates makes it easier to solve (by halving the problem dimension) as well as analyze (by revealing system invariants and frequencies). Unfortunately, determining a beneficial change of variables is often a challenging process requiring deep knowledge of the problem's underlying physical or mathematical structure. Many simulations may be using a suboptimal model formulation because a clever transformation has yet to be identified.

In this feasibility study, we affirmatively answered our feasibility question by showing machine learning and symbolic regression techniques can indeed be used to identify change of variables for certain classes of differential equations. We devised a numerical optimization procedure which parameterizes the change of variables using neural networks with special architectures to ensure invertibility properties. The networks are trained in a mesh-free way to reduce nonlinearity in a given differential equation. Finally, we postprocess the trained networks into interpretable symbolic expressions for the change of variables. Over the course of the feasibility study, we developed a Python library implementing this algorithm. On a suite of 12 test problems, it identified the correct change of variable on 10 which surpassed our feasibility threshold of a 50% success-rate. Additional research is needed to improve support and robustness for transforming independent variables, transformations with discontinuities and singularities, and vector-valued differential equations.

Mission Impact

Simulations involving differential equations crosscut the broad DOE/NNSA mission space. Advancements in how we formulate mathematical models enable more efficient and reliable predictions, and ultimately, can advance national security, energy, and scientific missions. This work contributes directly to the 3–5-year vision of enabling “new data-driven and AI-augmented approaches to scientific discovery” laid out in the LLNL 2025 Investment Strategy for Science and Technology. LLNL scientists and researchers can try our newly developed Python library to search for change of variables that improve their mathematical models. In the future, there is significant potential to build upon this foundational work and contribute to more sophisticated, multi-physics simulations used across the DOE.

25-FS-025: Target Design for Measuring the Opacity at White Dwarf Atmospheric Conditions

Project Overview

Recent observations from the Gaia survey have revealed an unexpected anomaly in the mass distribution of the oldest, coolest white dwarf stars, with those below 6,000K appearing significantly less massive than younger counterparts. This discrepancy challenges current models of stellar evolution and the age of the universe, suggesting a possible 60% error in the opacity models used to infer stellar masses. To address this, we attempted to design a multipass absorption cell experiment using a gas gun platform to directly measure the opacity of hydrogen gas under shock conditions. However, hydrodynamic and optical simulations showed that large (~10%) density fluctuations lead to uncontrolled beam refraction, making it infeasible to achieve the required measurement precision with our current design.

Despite this, the project provided valuable training opportunities for staff and students, and the results have clarified the limitations of our approach. Looking ahead, alternative experimental methods such as using cryogenic hydrogen targets may offer more promising avenues for probing high-density opacity effects. Additionally, further theoretical work to refine opacity calculations at extreme densities is essential to resolve the observed discrepancies in stellar models. By pursuing these experimental and theoretical paths, we can continue to advance our understanding of stellar physics and improve diagnostic capabilities for future research.

Mission Impact

This project addresses the High Energy Density Science Core Competency. Our goal was to design a new optical diagnostic platform for gases, enabling measurements of density, temperature, and constituents (atoms, molecules, and ions) that are crucial for understanding equation of state and reaction kinetics. Additionally, we aimed to create a new opacity platform capable of probing density effects to help interpret the significant (50%) discrepancies between measured and calculated iron opacities. After thorough evaluation, we found that measuring opacity with our current design is infeasible. This result indicates that alternative approaches should be pursued to address the identified challenges.

25-FS-026: Extending Generative Artificial Intelligence to Multi-Domain Deterrence

Project Overview

Identifying action-by-action escalation potential is a fundamental problem in strategic multi-objective games. Even in the single-objective case, effective decision-support in these games can be difficult: the space of potential scenarios is vast, simulation design is labor-intensive, and quantifying uncertainty for action-by-action escalation potential is challenging. These issues are exacerbated in multi-objective settings, where each action is a portfolio of multiple responses.

This LDRD Feasibility Study, proposed extending a new generative AI method, Generative Flow Networks (GFNs), to strategic interactions with multiple competing objectives under uncertainty. In this setting, GFNs first search on an action-by-action basis, then learn action-by-action probabilities of achieving the highest-benefit outcomes in a game. This key feature makes the approach interesting for many potential decision support tools.

In three stages, we extended a game-theoretic GFN called Adversarial Flow Networks (AFNs) to deterrence scenarios and classic game theoretic scenarios. Initially, AFNs only worked in simple games, but in head-to-head play they outperform AlphaZero, the famous DeepMind AI, and find more optimal strategies at a lower training cost. In Stage 1, we extended a public AFN codebase to play complete information, general-sum games and found that the AFN recovers optimal strategies (or, decision rules for best responses at any stage of the game). In Stage 2, we extended AFNs to more realistic scenarios, where agents may have incomplete information about the game or their opponent. We mathematically proved that AFNs, without an extension, cannot be applied to more complex games. From there, we developed a generalized AFN model called *Information Flow Networks* (IFNs). We tested them in classic incomplete information games, such as Kuhn and Leduc Poker, and found that IFNs perform as-good or better than state-of-the-art competitors. In Stage 3, blended our IFN with multi-objective learning methods to capture multi-objective strategies and study associations between strategies and outcomes. In summary, we found extending AFNs to deterrence is feasible and may offer a practical solution framework for decision support, new directions in scenario search, and action-by-action uncertainty quantification. By reaching our proposed extensions and confirming feasibility at all stages, IFNs may be a first step toward improving real-time decision support capabilities in multi-objective decision making.

Mission Impact

This feasibility study supports the Integrated Deterrence and Technology Competition Mission Focus Area addressing two key needs including developing deterrence metrics in extended or escalatory deterrence scenarios and developing a means of automated scenario design and setup to reduce workloads on human analysts. Having a model that provides approximate solutions in large, multiplayer strategic scenarios under various degrees of information and while balancing multiple objectives has significant potential for strategic and security capabilities. At tactical level, IFNs allow users to target approximate best responses to opponents, given preferences over multi-objective outcomes. At a strategic level, if there is knowledge about an opponent's preferences over multiple objectives, IFNs automatically allow users to target all possible strategies an opponent may

use and provide approximate best responses to each, without having to re-run any simulations. From the perspective of simulation design and analysis, IFNs may be able to dramatically prune down the space of possible scenarios one should consider, which would significantly reduce human effort in simulation design.

Publications, Presentations, and Patents

Artman, Conor, Nicholas Di, and Scott Perkins. "IFlowNets: Extending Generative Samplers to Learn Strategies in Incomplete Information Games." Workshop: Dynamics at the Frontiers of Optimization, Sampling, and Games @NeurIPS (2025): Accepted.

Artman, Conor, Nicholas Di, and Scott Perkins. "Extending Generative Flow Networks to Incomplete Information Games." NRO Forum for Innovative Research in Science & Technology (FIRST): Accepted.

Di, Nicholas, Conor Artman, and Scott Perkins. "IFlowNets: Extending Generative Flow Networks to Incomplete Information Games." *SIAM TXLA (2025)*: Accepted.

Artman, Conor. "Extending Generative Flow Networks to Incomplete Information Games." Center for Advanced Signal and Image Sciences (CASIS) Seminar Series.

Artman, Conor, Nicholas Di, and Scott Perkins. "Extending Generative Flow Networks to Incomplete Information Games." Poster Talk @ NRO Forum for Innovative Research in Science & Technology (FIRST): Accepted.

Artman, Conor, and Scott Perkins. 2025. "Report on Developing Information Flow Networks for Next Use Cases." Lawrence Livermore National Laboratory.

25-FS-031: Protein Engineering for Critical Metal Recovery Beyond Rare Earth Elements

Project Overview

Achieving decarbonization and electrification goals will require expanded production of critical minerals (CM), including Li, Co, Cu, rare earths, Ni, and graphite, whose supply chains are geopolitically vulnerable. Problematically, current extraction and separation processes pose severe environmental burdens that impede the development of a diversified domestic supply chain and undercut the environmental benefits of energy technologies. The development of efficient, economical, and environmentally sustainable processing technologies is thus important for meeting the CM demand of the emerging energy technology market. To this end, we have recently developed an all-aqueous protein-based process for rare earth element (REE) extraction and separation. To extend our protein-based approach to critical metals beyond REEs, the goal of this project was to develop a protein discovery and engineering pipeline to generate a panel of proteins that selectively bind target critical metals.

In this project, we adapted our SpyCI-LAMBS (SpyTag-Catcher Immobilization of Lanmodulins for Assaying Metal-binding Selectivity), which allows metal binding selectivity of metalloproteins to be assayed *en masse*, for use with metal ions beyond REEs. Specifically, we tested a panel of 70 natural and engineered proteins for binding to REEs, Indium (In^{3+}), and a panel of first row transition metals (Mn^{2+} , Fe^{3+} , Ni^{2+} , Co^{2+} , Cu^{2+} , Zn^{2+}). This led to the discovery that a natural REE-binding protein, which exhibits over a million-fold selectivity against alkaline earth metals and first row transition metals, bound In^{3+} with selectivity comparable to heavy REEs. Furthermore, substitution of specific active-site residues shifted selectivity for In^{3+} over a representative tightly binding REE, Pr^{3+} , by up to two-fold. These results suggest that this protein has the potential to enable efficient In^{3+} recovery from feedstocks such as end-of-life mobile-phone liquid crystal display screens, where high selectivity over Cu, Fe, Al, Mg, and Ni is paramount.

Mission Impact

Through expansion of our palette of CM binding proteins beyond REEs, we are working toward the development of a more efficient and sustainable process for CM recovery that can help alleviate the rapidly increasing CM demand (and associated supply vulnerability) for energy technologies. As such, this project is well-aligned with LLNL's mission area of "Energy Security" and the DOE's interest in establishing secure, domestic CM supply chains. The project also directly addressed the stated goals of the Bioscience and Bioengineering Division, including the development of advanced experimental systems that provide quantitative measurements for predictive models that advance the engineering of biomolecules for national security applications.

25-FS-032: Clouds and Precipitation over Urban Areas during Extreme Events and Climate Change

Project Overview

Urban areas, especially coastal cities, are experiencing dramatic impacts during the frequent occurrences of extreme weather events and will likely face challenges for future energy usage and infrastructure plannings. Clouds and precipitation and their coupling with urban land surface are very important physical processes to influence patterns and variabilities of the surface energy balance and water cycle. Such processes remain highly uncertain as traditional earth system models do not have adequate representations. The start-of-the-art numerical models with kilometer (or finer) resolution have great advantages by explicitly resolving convective motions in responses to urban settings at finer spatial scales. Hence, we will examine the model performance on representing this coupling process and provide assessment on model's increased strength and remaining deficiency for model improvement. This is an important knowledge gap to bridge so that we can trust these newly developed models in the resilience studies over urban areas.

This study includes evaluation of DOE's storm resolving model over urban and rural areas against available observations; and investigation of urban to rural differences varying with city sizes and with large-scale warming patterns. In a regional refined model simulations over California region, the simulated surface conditions such as air temperature are comparable with observations, however, large uncertainties exist considering differences between measurements over urban regions. In rural areas with grassland and forest land covers, the model shows moderate precipitation biases and high warm biases at surface. In present-day global simulations, the urban-rural difference in precipitation increases with city size, e.g. from small, medium, to large, then to mega-sized cities. While in a numerical experiment of uniform warming, such differences maintain similar levels and peak at medium to large cities but with a decrease in mega cities. These results suggest the need for more representative in-situ measurements over urban settings and the necessity to consider the impact of city size on urban-rural differences in precipitation and other meteorological conditions for the energy and infrastructure plannings.

Mission Impact

This study extends our research areas to urban impacts and prepares us for the DOE funding opportunities, e.g., Atmospheric System Research (ASR) and Earth & Environmental Systems Modeling (EESM), especially those related to recent and upcoming field campaigns over urban areas by DOE's Atmospheric Radiation Measurement (ARM) program.

This work bridges gaps in understanding urban environment, urban-rural difference, and their coupling with cloud and precipitation processes and their representations in DOE's newly developed global storm resolving model. This work aligns with the Earth and Atmospheric Science Core Competency and on physical process understanding and model improvements of the DOE EESM/ASR/ARM programs.

25-FS-033: Solving the Pulsed-Power Driven Inertial Fusion Energy Standoff Problem

Project Overview

The standoff problem in pulsed-power driven IFE (Inertial Fusion Energy) refers to the problem of electrically connecting a fusion target with the driver in a way that preserves the driver/target interface in the presence of a large fusion energy release (100's of megajoules to 1000 megajoules). High yield fusion drivers for stockpile stewardship applications have similar concerns, but without the complication of the high repetition rate needed for energy production. All proposed IFE or high yield systems have the challenge of protecting the reactor vessel and driver from the energy release, but pulsed power drivers have the additional challenge of establishing an electrical connection in a way that does not create excessive debris or require costly/massive structures that must be expendable. Fortunately, there are conceptual solutions in the form of very low mass transmission lines, usually in the form of wires or foils, since very little mass is needed to overcome the magnetic forces driving the transmission lines apart or provide a low resistance pathway given the short pulse duration of the driver.

Several important aspects of the standoff problem were analyzed in the course of this LDRD project. Conceptual means of introducing the low mass transmission lines into the reactor chamber were proposed, including analysis of methods to retain the power flow gap between the electrodes in the presence of the chamber environment. The energy losses due to ohmic dissipation and magnetic acceleration of the low mass transmission lines were evaluated for candidate driver pulses and different transmission line masses, and the fluence of x-ray and neutron energy on the persistent power flow structures that must survive the pulse of energy were evaluated. Finally, means of rapidly pumping down the chamber were explored as a way to return the system to low pressure following the multi-atmosphere post-pulse pressure rise. The overall conclusion from the analysis is that, while the reactor environment creates stressful conditions for a low mass transmission line standoff system, there are concepts expending 10 kg or less of electrode mass each pulse with the potential to mitigate the stresses and successfully drive fusion targets. Whether such a system could lead to a practical and economical fusion reactor would require extensive research and development beyond the scope of the feasibility study.

Mission Impact

LLNL is currently exploring ways to interact with the private sector on fusion energy research since the DOE is encouraging such interaction through the Fusion Innovation Research Engine (FIRE) and the Innovation Network for Fusion Energy (INFUSE) programs for example. Work in this area is synergistic with our ICF/weapons physics mission since the long-term goal of the ICF program is a high yield (GigaJoule-class) capability that must grapple with a number of similar issues as those found in IFE. The research pursued in this LDRD project could be a help to these new mission areas since it is establishing Laboratory capability in the technology of pulsed-power-based IFE, the primary focus of several IFE companies. The research also informs an eventual pulsed-power-based high yield driver, the ultimate goal of the Laboratory's magnetic direct drive program.

Record of Invention

IL 2025-317 "Concept for Low Mass Transmission Lines for Pulsed Power Fusion."

25-FS-034: Predictive Science-Based High Explosive Safety Feasibility Study

Project Overview

This project numerically investigates how different high explosive (HE) prill morphology and thermodynamics conditions influence its burning behavior. Two numerical solvers in LLNL's ALE3D were considered: (1) the explicit hydrodynamic solver and (2) the implicit Computational N-Fluid Dynamic (CNFD) solver. All simulations performed in this project were 2D axisymmetric. With the explicit hydrodynamic solver, we used a level set method to model the flame front at constant speed. Effects of different background pressure, HE prill shape and porosities, as well as flame speed on the burning behavior, were investigated. The baseline geometry is a 1-mm diameter spherical HE prill. When the entire prill surface is ignited, the effect of background gas pressure is minimal. However, when a 60-degree portion (arc-lighting) of the surface is ignited, the reaction is sufficient to cause particle motion in the absence of a restraining boundary condition. Additionally, arc lighting conditions and a reduced background gas pressure permits the ignition to spread and envelope the entire particle surface more quickly thus increasing the mass burn rate. Two different ellipsoidal shapes were then considered: an oblate spheroid, which elongates in the normal direction to the axis of symmetry; and prolate spheroid, which elongates through the axis of symmetry. These ellipsoids have the same mass, but 40% more surface area compared to the spherical prill. Like the spherical case, these prills were arc-lighted around the axis of symmetry. The oblate spheroid burns faster while the prolate spheroid burns slower than their spherical counterpart. While we did not calculate ellipsoidal shapes with full surface lighting, it is reasonable to assume that ellipsoids will increase the mass burning rate due in part to the increased surface area per unit mass relative to the sphere, and in part to a smaller distance from surface to the inner volume.

In the second part of this project, simulation of a 2-mm radius spherical prill surrounded by 800oC inert air was performed using CNFD. Air was injected from left to right at the speed of 1 mm/s, which means convective heat transfer dominates the left half of the prill compared to the right half. Therefore, the HE prill preferentially deflagrates on the left side. The flame then moves from left to right, eventually envelopes the entire HE particle. Such complex HE deflagration behavior has never been simulated using a Computational Fluid Dynamics (CFD) based code.

Mission Impact

This project is relevant to the Advanced Materials & Manufacturing Core Competency and the Nuclear Deterrence/Stockpile & Enterprise Transformation Mission Focus Area because it is aimed at enabling accelerated HE formulation efforts for agile nuclear deterrent, future stockpile, and Energetics 2040 goals.

22-LW-029: Nuclear Detective Work in the Early Universe: The Mysterious Origin of Protein-Rich Stable Nuclei

Project Overview

Neutron-induced reactions on unstable nuclei play a critical role in stellar nucleosynthesis. While we have understood the basics of stellar nucleosynthesis for nearly 70 years, the production of some of the most proton-rich stable isotopes of certain elements continues to elude us. Researchers have proposed that such nuclei could be made in the neutrino-p process, which is thought to occur in the neutrino-driven winds which buffet and disperse the material created in a core-collapse supernova. However, whether these mysterious isotopes can be created in the neutrino-p process depends on the relative speed of creation (predominantly neutron-induced) and destruction (mostly proton- or alpha-induced) reactions on certain short-lived nuclei. The proton- and alpha-induced reactions are well constrained, so uncertainties in the neutron-induced reactions (the most important of the neutron-induced reactions are (n,γ) and (n,p)) dominate the nuclear physics uncertainties in nucleosynthesis models. Making the picture even more complicated, these nuclei are too short-lived for direct measurements. This project used an indirect technique, called the Surrogate Reaction Method (SRM) to answer this question. First, we made a measurement to benchmark the SRM for (n,p) reactions, which had never been done, and second, we made a measurement to constrain (n,γ) and (n,p) on ^{62}Zn , an important nucleus in neutrino-p process nucleosynthesis.

Mission Impact

This project made two important contributions to the mission of Lawrence Livermore National Laboratory (LLNL). First, we have provided the data which we need to extend the SRM to constraints of (n,p) reactions. In addition to playing an important role in nucleosynthesis, these reactions are important for a variety of applications relevant to Stockpile Stewardship. Second, we have demonstrated, for the first time, the impact of Machine Learning (ML) techniques in background reduction for SRM experiments.

Publications, Presentations, and Patents

In, Eun Jin, Emanuel Chimanski, Jutta Escher, Sophie Péru, Aaina Thapa, and Walid Younes. "Electric Dipole Excitations near the Neutron Separation Energies in ^{96}Mo ." *EPJ Web of Conferences* 322 (2025): 04003. <https://doi.org/10.1051/epjconf/202532204003>

Ghimire, R., A. Ratkiewicz, S. D. Pain, K. A. Chipps, J. A. Cizewski, K. L. Jones, P. Bedrossian, et al. "Background Subtraction in Inelastic Scattering Measurements Using Machine Learning." *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 561 (April 2025): 165649. <https://doi.org/10.1016/j.nimb.2025.165649>

Escher, Jutta, Kirana Bergstrom, Emanuel Chimanski, Oliver Gorton, Eun Jin In, Michael Kruse, Sophie Péru, et al. "Improving Nuclear Data Evaluations with Predictive Reaction Theory and Indirect Measurements." *EPJ Web of Conferences* 284 (2023): 03012. <https://doi.org/10.1051/epjconf/202328403012>

Matthew Williams, "Demonstrating inelastic proton scattering as a surrogate for (n,g) and (n,n'g)" (poster presentation, Postdoc Poster Symposium, Livermore, California, May 3, 2023).

Matthew Williams "Experimental Studies on the Nuclear Fingerprints of Massive Stars" (invited presentation, i-process workshop 2023, Poseidonia Beach Hotel, Limassol, Cyprus, May 19, 2023).

23-LW-014: Engineering *Bacillus Subtilis* for Controlled Gaseous-Nitrogen Fixation to Reduce Artificial-Nitrogen Use and Enhance Microbial-Community Function

Project Overview

Chemical nitrogen fertilizers have become a critical component for agriculture production. However, these fertilizers have important drawbacks including negative water supply impact from eutrophication, demand on power grids, and reliance on global supply chain which can be disrupted by geopolitical tensions especially with Russia and China producing at least 25% of all chemical fertilizers. The Haber-Bosch process generates chemical nitrogen fertilizers requiring 2% of the global energy supply to meet demands. Notwithstanding, these fertilizers are marginally effective at delivering nitrogen to the plants as 50% is lost to runoff and back into the air as pollutants. Ultimately, a solution is needed to sustain agriculture as the global population increases while eliminating these drawbacks from chemical fertilizers and that is where microbial communities that are enhanced can provide this solution. Yet, enhancing microbial communities by adding biofertilizers (BFs, microbes that provide nutrients to the plant) or biostimulants (microbes or molecules that stimulate plant performance/resilience) to increase plant performance has been problematically inconsistent due to poor persistence in soil, unknown impact on the soil microbiome and variation between plant hosts leading to low adoption by growers especially in the US. Accordingly, this project aimed to provide a high-throughput, automation-compatible pipeline for testing how a BF might persist with, improve, or disrupt soil microbial communities plus demonstrate how BFs could be designed to deliver nutrients to the plant when there is key abiotic stress for the plant while improving microbial fitness during the nutrient delivery process. Lastly, as an outgrowth of the effort, this foundational work helped establish a collaboration with the National Agriculture and Food Research Organization (NARO) of Japan that sparked a plus-up effort related to utilizing BFs from LLNL and NARO to increase soybean performance and utilize computational modeling to make predictions about BF efficacy with increasing plant performance in the field.

To tackle the challenges and accomplish the aims established above, the project set out to establish the high-throughput pipeline for testing BF interaction with other microbes and engineering new abiotic (temperature and salinity) stress responsive BFs to deliver nitrogen to plants in parallel. For the microbial interaction pipeline, the BF organism used for nitrogen delivery was engineered to produce a response that would allow for simplistic, high-throughput tracking while interacting with complex groups of microbes. Furthermore, microbes from various soils were cultivated so microbial communities could self-assemble from the soil under various conditions which provided a representation to test the BF interaction and capability to persist. After testing the capability to track the BF and exploring how the BF interacted with microbial communities, the microbial interaction pipeline was established and published in *The ISME Journal* which generated interest from the private sector at the 9th Microbiome AgBioTech Summit. For creating new BFs that respond to plant stress conditions when delivering nitrogen, a well-established BF organism that consistently supports plants and was also used in the interaction pipeline was genetically engineered to fix gaseous nitrogen in response to temperature and salinity increase as a proof-of-principle around using these stressors as a trigger for nitrogen delivery when the plant needs nitrogen the most. The new BFs successfully fix nitrogen which was determined by tracking isotopically labeled nitrogen gas using a LLNL special capability, Nanoscale Secondary Ion Mass Spectrometry (NanoSIMS).

Additionally, using the genetic switch concept that responds to temperature and salinity, the BFs growth and viability significantly improved compared to the original BF organism when depleted of non-gaseous nitrogen and the genetic switches showed promise in delivering nitrogen but maintaining viability of the BFs when exposed to lower temperatures and salinity which was an important goal. Accordingly, this emphasized the need to test the BFs with a plant host such as corn in greenhouse experiments. This stimulated a collaboration with Ginkgo Bioworks to provide state-of-the-art greenhouse facilities to evaluate the BFs. Concurrently, these successes prompted the outgrowth of the work into the collaboration with NARO of Japan. Leveraging the new collaborations with Ginkgo Bioworks and NARO, a new aspect of the project was begun to apply BFs from both LLNL and NARO in combination (elucidated as a possibility from some literature but more confirmed by the microbial interaction pipeline results) to improve soybean performance which will be maximized by utilizing computational modeling at LLNL to disentangle of the complexities of agriculture. Correspondingly, the nitrogen delivery BFs and soybean BFs were tested in the greenhouse for improving plant performance throughout the recent summer months with promising data being analyzed. Ultimately, the nitrogen delivery BF success is culminating into a manuscript that will be published with the support of a new nitrogen bioimaging project supported by DOE Biological and Environmental Research (SCW1904) because the nitrogen delivery BFs will be utilized on this new project and the soybean BF efforts with NARO is being continued as a newly funded project at LLNL (26-ERD-006).

Mission Impact

Food security has classically been viewed as a non-issue in the US but recent reports such as the report from the National Security Commission on Emerging Biotechnology begins to highlight the sense of urgency to consider food security as part of the national security umbrella even in the US. Food production in the US is heavily reliant on imported chemical fertilizers from peers such as China and Russia which could cripple US food production if supply is diminished which draws parallels between food security and the critical materials space. Accordingly, multiple agencies such as DARPA and ARPA-E have developed programs in the current and recent years to start developing biotechnology to address the food security challenge. Additionally, venture capitalist investment has sparked growth in the agricultural biotech space over the last decade, but this support of the private sector has waned due to the minimal adoption by growers. Therefore, LLNL has a unique opportunity to engage on food security as it starts to become national security and bolster the private sector to create real change. This project created the foundation needed to maximize this opportunity. This project has started to build a network of collaborations in agriculture that includes the private sector, academic institutions, agriculture outreach and research extension centers that interface with growers, and an international collaboration with Japan (NARO). The project continues to expand the research directions of LLNL by expanding into the applied biotechnology space for agriculture which will recruit new talent while leveraging current capabilities such as computation to tackle the food security (food production) challenge. Ultimately, this project demonstrated that LLNL can develop tools to improve biotechnology for agriculture, expand into a new research space that will be part of the future national security mission, and that current capabilities such as computation power can be brought into the food security space which is essentially bridging computation and agriculture so in California could appear as LLNL bridging the Silicon and Central Valleys.

Publications, Presentations, and Patents

Madsen, Cody S., Kimbrel, Jeffrey A., Diep, Patrick, and Ricci, Dante P. 2025. "Synthetic communities as a model for determining interactions between a biofertilizer chassis organism and native microbial consortia." *The ISME Journal* 19, no. 1 (August).
<https://doi.org/10.1093/ismejo/wraf170>. LLNL-JRNL-2002743.

Madsen, Cody S., Kimbrel, Jeffrey A., Diep, Patrick, and Ricci, Dante P. 2025. "Synthetic communities as a model for determining interactions between a biofertilizer chassis organism and native microbial consortia." (Poster Presentation at 9th Microbiome AgBioTech Summit, Raleigh North Carolina, August). LLNL-POST-2010055.

Madsen, Cody S., Kimbrel, Jeffrey A., Diep, Patrick, and Ricci, Dante P. 2024. "Advancing nitrogen biofertilizers to reduce the utilization of the Haber-Bosch process." (Poster Presentation at LLNL postdoc poster session, Livermore California, July). LLNL-POST-867655.

Madsen, Cody S., 2025, "Strengthening Food Security: Integrating Biofertilizers and Computational Modeling for Sustainable Agriculture." (Presented at Visit from Mr. Shigeharu Aoyama and Consulate General of Japan, Livermore California, August 2025).

Madsen, Cody S., 2025, "Strengthening Food Security: Integrating Biofertilizers and Computational Modeling for Sustainable Agriculture." (Presented at Visit of LLNL to National Agriculture and Food Research Organization of Japan, Virtual, July 2025).

Madsen, Cody S., 2024, "Towards predictive computational models for agriculture: how modeling plant-microbe interactions, climate conditions and agriculture parameters could increase food security, agricultural performance and soil health." (Presented at Visit from the National Agriculture and Food Research Organization of Japan, Livermore California, November 2024).

Madsen, Cody S., 2024, "Advancing nitrogen biofertilizers to reduce the utilization of the Haber-Bosch process." (Presented at LLNL postdoc seminar, Virtual, July 2024).

Madsen, Cody S., 2024, "Utilizing *Bacillus subtilis* for enhancing understanding of microbial community dynamics and controlled nitrogen fixation to reduce demand for chemical nitrogen fertilizers." (Presented at Invited seminar for meeting with National Agriculture and Food Research Organization of Japan, Virtual, March 2024).

23-LW-016: Manipulating the Spin of Nuclei with Nuclear Reactions

Project Overview

Magnetic moments of nuclei in short-lived excited states are excellent probes of nuclear structure and reaction dynamics, but they are extremely difficult to measure because they require spin-polarized nuclei that must be generated during the reaction itself. Recent work by our team identified a promising mechanism in inelastic nuclear scattering that can create strong spin alignment in the reaction products, potentially unlocking magnetic-moment measurements that have been out of reach. We designed and fielded a proof-of-principal experiment at Argonne National Laboratory's ATLAS facility using the Gammasphere high-purity germanium array. With a carbon beam on a carbon target, we populated the well-known first excited state of carbon-12 and recorded the emitted gamma rays with Gammasphere while tagging the scattered particles with auxiliary detectors. By observing the dependence of the gamma-ray emission on scattering angle and beam energy, we can map the onset and magnitude of polarization predicted by our reaction model. The central experimental run has been completed, and the preliminary analysis indicates that spin-alignment was generated in line with our predictions. Completing the Gammasphere run provides the high-statistics, angle-resolved gamma-ray data we need to validate our reaction models that describe the spin polarization of excited nuclei. This work lays the foundation for new magnetic moment measurements of excited nuclei, including on exotic isotopes, at ATLAS or other facilities such as the Facility for Rare Isotope Beams.

Mission Impact

This project advances LLNL's core competency in nuclear science and measurement by developing a practical method to create and diagnose spin-polarized excited nuclei—improving the fundamental data and models that underpin nuclear structure, reactions, and related applications. The capability supports NNSA missions by enhancing science and technology tools relevant to national security and by enabling new ways of responding to future challenges. This project also strengthens partnerships and workforce pipelines with U.S. user facilities (ANL/ATLAS) and universities. The successful demonstration of the spin-polarization mechanism also presents the opportunity for a new research direction at LLNL to perform magnetic-moment measurements of short-lived states, with near-term opportunities to integrate the method into future experimental campaigns.

24-LW-003: Origins of the Solar Boron Isotope Ratio: Insight into Nucleosynthesis in the Neutrino Process and Low-Energy Charged Particle Irradiation

Project Overview

The difference in boron isotopic compositions between the Solar System ($^{11}\text{B}/^{10}\text{B} = 4$) and Galactic Cosmic Rays (GCRs, $^{11}\text{B}/^{10}\text{B} = 2.5$) is a long-standing astrophysical conundrum. This discrepancy suggests the presence of an additional source of ^{11}B . To identify the source of this extra ^{11}B , we developed a new high-spatial-resolution ion imaging method using the LLNL NanoSIMS 50 to search for isotopically anomalous Li- and B-bearing components in primitive carbonaceous chondrites. Our search identified grains with elevated $^{11}\text{B}/^{10}\text{B}$ ratios. Due to the small size of the carrier grains, mixing calculations suggest their true ratio could be >10 , a value outside the range produced by low-energy spallation. This finding points to a neutrino-spallation origin, implying that supernovae may be the source of the excess needed to produce the solar system's B isotopic ratio.

Mission Impact

The discovery of high $^{11}\text{B}/^{10}\text{B}$ ratios will result in high-impact publications, new funding opportunities, and programmatic benefits. One manuscript on the long-standing B isotope problem, our overarching goal, is being written up and very close to submission to Nature Astronomy. The publication will be of great interest to not only cosmochemists but also to astrophysicists, especially those working on nucleosynthesis theories and star formation. The methods developed for this work are highly relevant to our nuclear forensics work, demonstrating our ability to measure light isotopic ratios in sub-micron targets. We can use these methods to partially support the existing R3 (rapid-response research) NNSA venture focused on post-detonation nuclear forensics (K. Knight and T. Parsons-Davis) and apply for additional NNSA funding to develop these signatures for pre-detonation nuclear forensics.

Presentations

McCain, K. A. and Liu, M.-C. 2024. "Diverse Nucleosynthetic Heritage of Li-rich Material in the CO3.05 Chondrite NWA 7892." 86th Annual Meeting of the Meteoritical Society, abstract #6426 (LLNL-ABS-864307; LLNL-PRES-866876).

McCain, K. A. and Liu, M.-C. 2025. "Towards Understanding Li and B Isotopic Anomalies in Primitive Carbonaceous Chondrites." 87th Annual Meeting of the Meteoritical Society, abstract #5282 (LLNL-ABS-2005299; LLNL-PRES-2008116).

24-LW-006: Designing Robust Bioproduction Bacteria for Use in Non-Sterile Bioreactors

Project Overview

Bacterial chemical production (biosynthesis) can replace current chemical synthesis processes that produce greenhouse gas emissions, toxic waste, and non-biodegradable end products. However, widespread adoption of biosynthetic processes is hindered by the high risk of contamination of entire bioreactors (100 – \geq 100,000 liters), which results in profit loss and reduces the market competitiveness of biotechnology. To increase biomanufacturing competitiveness, we set out to engineer a bioproduction strain (e.g., *Pseudomonas putida*) to withstand pH levels that would inhibit contamination (>9) at bioreactor scale. To this end, we identified portable (i.e., useful for bioengineering) pH tolerance genes by applying both computational and experimental strategies and leveraging the industrially relevant, genetically diverse genus *Pseudomonas*. Our approach combines: 1) intra-genus comparative genomics, 2) a randomly barcoded transposon library (RB-TnSeq), and 3) transcriptomics (RNA-seq) in a facultative alkaliphile. Our pan-genome analysis of *Pseudomonas* identified 194 core gene families specific to Gram-negative alkaliphiles. We find that the most alkaliphile-enriched gene families influence lipid metabolism, secretion and motility, signal transduction, protein folding, and secondary metabolite production. With TnSeq we discovered a global transcriptional regulator likely responsible for facilitating physiological adaptation to alkaline pH in *P. alcaliphila*. Then, using RNA-seq, we determined that those adaptations involve outer membrane reorganization, lipid biogenesis, ion transport, and alternative energy generation pathways. Collectively, our results reveal that alkalitolerance in Gram-negative bacteria is encoded primarily in stress response pathways and is therefore an ideal bioengineering tool. Additionally, because our experimental results largely agree with our bioinformatic findings, we believe this computational workflow can be used more broadly to discover genes associated with any trait of interest, given the existence of related strains both with and without the phenotype. This study significantly advances our understanding of how facultative alkaliphiles alternate between growth at neutral and alkaline pH. Through this analysis, we have successfully discovered gene candidates and genetic pathways for bioengineering of synthetic alkaliphiles.

Mission Impact

The results of this project support LLNL's Bioresilience Mission Focus Area and Biosciences and Bioengineering Core Competency by contributing fundamental research to the development of a novel biotechnology that will strengthen U.S. supply chains and position the U.S. as a leader in advanced biotechnology research & development. Additionally, this project addresses DOE-BTO's Bioproduct Production and Waste-to-Energy program areas, with recent funding calls reflecting a focus on developing renewable chemicals and biofuels. Therefore, our work positions LLNL for future DOE-funded projects involving circular bioprocess design to address DOE's energy and environmental security missions. The RB-TnSeq library we designed in a facultative polyextremophile is now a resource for future work in BBTD; it enables the exploration of salt, cold, and pH tolerance in an industrially relevant bacterial genus. This work has created new opportunities for cross-institutional collaborations (e.g., LBNL, NASA, Pioneer Labs) towards experimental engineering of synthetic polyextremophiles for use throughout the bioeconomy and for future space travel and terraformation.

Publications, Presentations, and Patents

Christina, K.Y. and Halvorsen, T.H. “Designing a synthetic alkaliphile to increase bioreactor efficiency for more affordable biomanufacturing.” Society for Industrial Microbiology (SIMB) Annual Congress, San Francisco, CA, 2025. LLNL-POST-2007809

Christina, K.Y. and Halvorsen, T.H. “Designing a synthetic alkaliphile to increase bioreactor efficiency for more affordable biomanufacturing.” Federation of European Microbiologists (FEMS) Annual Congress & Exhibition, Milan, Italy, 2025. LLNL-CFPRES-2011797

24-LW-015: Addressing Rare-Earth Supply Challenges with New Production Methods for Cerium–Iron–Nitrogen Permanent Magnets

Project Overview

The global shift toward renewable energy and electrified transportation is increasing demand for permanent magnets, which are essential for technologies such as electric vehicles and wind turbines. Currently, the most widely used permanent magnets rely on rare earth elements like neodymium, which are scarce and largely processed outside the United States, posing a significant supply risk. This project aimed to develop a new class of permanent magnets based on the more abundant elements cerium, iron, and nitrogen, specifically targeting the CeFe₁₂-type structure and its nitrided forms. The goal was to create alternatives to current magnets that reduce reliance on critical rare earth elements.

To address this need, the team mapped the phase stability of the CeFe₁₂-xTi_x system, optimized the composition and processing parameters, and developed advanced densification methods such as spark plasma sintering and selective laser melting. The project successfully synthesized the pure CeFe₁₂-xTi_x magnet phase, established the processing conditions for nitriding and sintering of powders and characterized the magnetic properties. The results form a foundation for the development of CeFe₁₂N-type magnets by focusing on realistic manufacturing pathways and thereby laying the groundwork for a more resilient domestic supply chain for permanent magnets.

Mission Impact

This research supports the mission of Lawrence Livermore National Laboratory to advance materials science for national security and energy resilience. By developing new processing methods and understanding the properties of Ce-Fe-N magnets, the project provides a foundation for alternatives to critical-element-based magnets, which is relevant to the missions of the Department of Energy. The knowledge and techniques developed are also transferable to other advanced manufacturing and materials programs, enabling new research directions and collaborations.

Publications

Amon, Alfred, and Scott McCall. 2025. "Opportunities for Cerium valorization in the Rare Earth supply chain." In Proceedings of TMS 2025, Las Vegas, NV, March. LLNL-PROC-869254.

Kim, Eunjeong, Alexander Wilson-Heid, Joe Boro, Alexander Baker, Ashley Lee, Martin Kunz, and Alfred Amon. 2025. "The Ce-Fe-Ti System: Phase Equilibria in the Fe-rich Corner at 1000 degrees Celsius." *Journal of Phase Equilibria and Diffusion* 46: 299-306. <https://doi.org/10.1007/s11669-025-01195-2>. LLNL-JRNL-872240.

Presentations

Amon, Alfred, Eunjeong Kim, Alexander Wilson-Heid, Alexander Baker. 2024. "Advanced Processing Methods for CeFe12-Based Permanent Magnets." Presented at MRS Fall Meeting 2024, Boston, MA, December 2024.

Amon, Alfred, Eunjeong Kim, Alexander Wilson-Heid, Alexander Baker. 2025. "Advanced Processing Methods for CeFe12-Based Permanent Magnets." Presented at TMS 2025 Annual Meeting and Exhibition, Las Vegas, NV, March 2025.

Amon, Alfred, Eunjeong Kim, Alexander Wilson-Heid, Alexander Baker. 2024. "Laser Processing of Ce-Based Permanent Magnets to Support the Domestic Magnet Supply Chain." Presented at MS and T 2024, Pittsburgh, PA, October 2024.

Amon, Alfred. 2025. "Opportunities for Cerium Valorization in the Rare Earth Supply Chain." Presented at TMS 2025 Annual Meeting and Exhibition, Las Vegas, NV, March 2025.

Amon, Alfred. 2024. "Opportunities for Cerium Valorization in the Rare Earth Supply Chain." Presented at MRS Fall Meeting 2024, Boston, MA, December 2024.

24-LW-020: Giant Superconducting Diode Effect in Emerging Quantum Materials

Project Overview

Modern quantum technologies, such as quantum computers and sensors, require highly efficient electronic circuits that minimize energy loss. To achieve this, it is crucial to develop materials that allow current to flow preferentially in one direction without dissipation—a phenomenon known as the superconducting diode effect. Our research was motivated by the need for game-changing advancements in non-dissipative electronic circuits, which could dramatically improve the performance and energy efficiency of next-generation quantum devices.

To address this need, we focused on using emerging topological materials to engineer systems that exhibit a giant superconducting diode effect. By designing, fabricating, and testing these materials, we were able to identify conditions under which supercurrent flows preferentially in one direction. The successful realization of these superconducting diodes demonstrates a new functionality for electronic circuits and opens the door to transformative advancements in superconducting electronics. This work not only advances fundamental understanding of novel quantum materials but also lays the groundwork for more energy-efficient and scalable technologies in the quantum industry.

Mission Impact

Realizing a giant supercurrent diode effect on a scalable platform offers multiple mission benefits. This research advances the scalability and versatility of electronic devices by enabling energy-efficient superconducting electronics, supporting LLNL's goal of driving innovation in high-performance technologies. With only a few candidates of nonreciprocal superconducting materials currently known, the prediction, synthesis, and characterization of such systems open new research directions and address fundamental questions in condensed matter physics. The project strengthens LLNL's leadership in quantum materials, contributes to defense technology innovation, and expands capabilities in superconducting device development, while also advancing DOE/NNSA missions and aligning with the interests of other federal agencies.

Publications, Presentations, and Patents

Enrico Rossi, Joseph J. Cuzzo, Dong-Xia Qu, Javad Shabanid, and Wei Pan, "Shapiro Steps and Microwave Tunable Diode Effect in Novel Josephson Junctions," Proc. SPIE 13119, *Spintronics* XVII, 131190I (2024). LLNL-PROC-2011726

Nick Du, Jenny Zhou, and Dong-Xia Qu, "Characterization of polarity-reversible Nb/Pt Josephson supercurrent diodes," APS Global Physics Summit, Anaheim, CA, March 19 (2025). LLNL-PRES-2003718

Maxwell Stafford and Dong-Xia Qu, "Synthesis and Characterization of Superconductor Diodes," LLNL Summer Intern Presentation (2024). LLNL-POST-868822

Maxwell Stafford and Dong-Xia Qu, "SULI Report Synthesis and Characterization of Superconductor Diodes," SULI Summer Intern Report (2024). LLNL-TR-868821

Dong-Xia Qu, J. Cuzzo, N. Teslich, K. Ray, Z. Dai, T. Li, G. Chapline, J. DuBois, E. Rossi, "Phase-Slip Lines and Anomalous Josephson Effects in Tungsten Nanoscale Cluster-Based Topological Insulator Nanobridges: Implications for Topologically Protected Qubits and Quantum Sensors," *ACS Appl. Nano Mater.* 23, 3702 (2024). LLNL-JRNL-843054

24-LW-026: Relating Oxidative Protein Damage to Antioxidant Status in Health and Disease

Project Overview

Antioxidant supplements are widely used to protect health, yet some studies suggest they can sometimes worsen disease, including certain cancers. We set out to clarify how antioxidants affect the body's chemistry, especially markers of oxidative damage, so that patients, clinicians, and public-health agencies can make better, evidence-based decisions.

We pursued two complementary strategies. First, we characterized an ultra-sensitive tracing method that pairs accelerator mass spectrometry with high-resolution mass spectrometry (PAMMS) to follow how chemicals are processed in the body; this validated LLNL's ability to detect and identify trace metabolic products in blood with exceptional sensitivity. Second, we profiled blood from a controlled mouse study using untargeted metabolomics, a discovery approach that scans broadly for changes across hundreds to thousands of small molecules without preselecting targets. This work, enabled by LLNL's new Orbitrap Eclipse instrument, revealed clear, statistically significant differences between diet and disease groups: dozens of blood chemicals shifted when cancer-bearing mice were fed high-antioxidant diets compared with normal diets. Together, the results show that antioxidant intake can substantially reprogram systemic metabolism in a cancer context and establish two powerful LLNL capabilities, PAMMS tracing and untargeted metabolomics, for future health-security, exposure, and translational studies. These tools now position LLNL to support evidence-based guidance on supplement use, assess health impacts of environmental exposures (e.g., wildfire smoke), and collaborate with agencies and industry on next-generation biomarker development.

Mission Impact

This project advances LLNL's core national security mission, with direct impact on Health Security and chemical and radiological consequence management, by delivering a dual capability for chemical-exposure forensics and health-relevant phenotyping: (1) PAMMS-enabled radiocarbon tracing coupled to high-resolution Orbitrap LC-MS for ultra-sensitive identification and quantification of xenobiotic metabolites, demonstrated with wood-smoke catechol, leveraging LLNL's Biological AMS (BioAMS); and (2) a discovery-scale metabolomics workflow on the new Orbitrap Eclipse that reveals redox and lipid-signaling rewiring in tumor-bearing hosts under antioxidant diets. Together these establish cornerstone methods for an LLNL metabolomics core, expand BioAMS integration with molecular MS, and seed cross-directorate programs spanning Physical and Life Sciences and Global Security in exposure assessment, biomarker discovery, and precision toxicology. This work directly advances the LLNL Biological Mission Focus Area, providing mission-relevant analytical platforms and datasets for exposure attribution, mechanistic toxicology, and precision health assessments, and enabling execution of bioMFA use cases in wildfire smoke and industrial-release exposure assessment and consequence management in partnership with BioAMS and the Forensic Science Center. The results directly support DOE/NNSA priorities in health security, readiness, and consequence management, enabling rapid attribution of exposures, mechanistic risk assessment, and decision support during environmental or radiological incidents, and align with DOE Office of Science's Biological and Environmental Research on

systems-level responses to stressors. They also create clear on-ramps for external programs at NIH, NCI, NIEHS, EPA, CDC, DOD, DTRA, and DHS, while attracting collaborations and staff to grow LLNL's analytical and translational biosciences portfolio.

Publications, Presentations, Patents

Baliu-Rodriguez, David, Dorothy J. You, Michael A. Malfatti, Esther A. Ubick, Bruce A. Buchholz. "Identification and Quantitation of ¹⁴C-Labeled Catechol Metabolites in Rat Plasma after Intranasal Instillation of Smoldering Eucalyptus Wood Smoke Extract." Poster Presentation, Mass Spectrometry & Advances in the Clinical Lab Annual Conference, Montreal, CA, September 2025.

24-LW-035: First Demonstration of Continuous Gigahertz-Terahertz Radiation by a Reversible Phase Transition

Project Overview

The project we have conducted focuses on the first demonstration of gigahertz–terahertz (GHz–THz) electromagnetic (EM) radiation generated by an ultrafast laser-induced magnetic phase transitions in ferromagnetic materials such as iron, nickel, and cobalt. One of the primary motivations for this work is the current lack of high-power (specifically, mW-level) GHz–THz sources, which prevents many of their promising applications from becoming practical in areas such as biomedicine, materials characterization, and next-generation telecommunications. At present, most GHz–THz EM radiation sources rely either on ultrafast carrier dynamics in semiconductors, such as hole–electron recombination under an electric field, or on optical rectification in nonlinear optical crystals. However, there remains a significant gap in generating high-power GHz–THz radiation from ferromagnetic materials using their magnetic properties rather than electronic or optical ones. We proposed that, analogous to the mechanism of time-varying electric polarization in electronic materials and optical crystals, time-varying magnetic dipole moments can also generate GHz–THz electromagnetic fields. The main strength of this method is that, unlike the skin-depth limitations of semiconductors for GHz–THz generation and the low damage thresholds of conventional nonlinear optical crystals, bulk ferromagnetic materials exhibit much higher damage thresholds while maintaining accessible bulk properties. Harnessing the robust structural and magnetic properties of these materials presents a significant advantage. Moreover, we found that by controlling the temperature and pressure of these materials, we can achieve even higher peak intensities, which could form the basis of our next project, unlocking untapped possibilities for high-power (mW-level) GHz–THz sources. Once this power level is realized, it could have a direct impact on a wide range of technologies in biomedicine and national security, enabling applications such as concealed fentanyl detection, amyloid fibril detection, agricultural monitoring, and beyond.

Mission Impact

The development of GHz–THz light sources based on ultrafast lasers and ferromagnetic materials advances the fundamental understanding of light–matter interactions in laser and optical physics, as well as ultrafast magnetic domain interactions in ferromagnetic and emerging spintronic materials. Consequently, this work is expected to enhance our comprehension of spintronics, photon–phonon-related materials characterization, and the development of new optical instrumentation based on ultrafast lasers. These technologies also have practical applications in the detection and mitigation of high explosives and controlled substances such as fentanyl, addressing threats across a broad chemical and biochemical spectrum. Moreover, they strengthen the nation’s ability to protect critical infrastructure against chemical, biological, and natural hazards, while enabling the National Nuclear Security Administration (NNSA) to develop new strategies for responding to emerging national security challenges.

Publications

Choi, Wonjin, Sang Hyun, Minjeong Cha, and Nicholas Kotov. 2024. "Chiral Kirigami for Bend-Tolerant Reconfigurable Hologram with Continuously Variable Chirality Measures." *Advanced Materials*. <https://doi.org/10.1002/adma.202401131>. LLNL-JRNL-845947.

Chae, Soosang, Wonjin Choi, Lisa Nebel, Chang Hee, Quinn Besford, André Knapp, Pavlo Makushko, Yevhen Zabala, Oleksandr Pylypovskiy, Min Woo, Stanislav Avdoshenko, Oliver Sander, Denys Makarov, Yoon Jang, Andreas Fery, Jin Young, and Taeil Lee. 2024. "Kinetically controlled metal-elastomer nanophases for environmentally resilient stretchable electronics." *Nature Communications*. <https://doi.org/10.1038/s41467-024-47223-6>. LLNL-JRNL-845946.

Choi, Wonjin, Michael Armstrong, Jae Hyuck, and Taeil Lee. 2024. "Toward high-power terahertz radiation sources based on ultrafast lasers." *Journal of Materials Chemistry C*. <https://doi.org/10.1039/D4TC01502A>. LLNL-JRNL-862523.

Kwon, Junyoung, Jaebum Jeon, Mingu Lee, Serin Jeong, Wonjin Choi, Kyungmin Kim, and Jihyeon Yeom. 2025. "Enantioselective Se lattices for stable chiroptoelectronic processing media." *Nature Communications*. <https://doi.org/10.1038/s41467-025-59091-9>. LLNL-JRNL-2005356.

Choi, Wonjin, Ji-Young Kim, Myonghoo Hwang, Chungman Lim, Bumchul Park, Ahmet Emre, Sanghyun Lee, and Nicholas Kotov. 2025. "Highly Elliptic Circular Dichroism of Copper Aspartate One-Dimensional Nanostructures across the Ultraviolet to Terahertz Ranges." *Nano Letters*. <https://doi.org/10.1021/acs.nanolett.5c00411>. LLNL-JRNL-872303.

Chae, Soosang, Wonjin Choi, Su-Hyeong Lee, Quinn Besford, and Andreas Fery. 2025. "Tunneling Barrier-Integrated Gold Nanofilms for Negative Strain Gauging with Near-Zero Energy Consumption." *Nano Letters*. <https://doi.org/10.1021/acs.nanolett.4c06365>. LLNL-JRNL-871474.

Records of Invention

Choi, Wonjin, Mike Armstrong, Songyun Gu, Widi Moestopo, and Xiaoxing Xia. 2025. "Encrypted Chiral Holograms using Helical Photonic Metamaterials." 2025-221.

24-LW-037: Spooky Nuclear Fission: A Laboratory for Quantum Entanglement Studies

Project Overview

Quantum entanglement, the phenomenon by which properties of one particle can depend on properties of another particle, no matter how far apart they are from one another, is the most puzzling effect predicted by quantum mechanics; yet, it is at the heart of emerging quantum technologies, including quantum computing, quantum communications and quantum sensing. Somewhat surprisingly, the fragments resulting from the fission of a heavy nucleus could be a good example of a strongly entangled quantum, many-body system. However, no one has ever tested this hypothesis despite its possible consequences for the many applications of nuclear fission, ranging from applied physics such as carbon-free energy production or nuclear stockpile stewardship, to basic science through the role of fission in the formation of the elements in the universe and in driving the stability of super-heavy elements at the end of the periodic table.

The goal of this project was to develop a novel approach leveraging state-of-the-art nuclear Density Functional Theory (DFT) already implemented at LLNL to provide the first quantitative estimate of the degree of quantum entanglement (or entanglement entropy) between fission fragments. To this end, we first developed a new formalism to assess the impact of quantum correlations between fragments on observable quantities, taking as initial example the number of particles in the fragments. We found that the impact of these correlations was different depending on the fragmentation mode of the fissioning nucleus (nearly equal fragments or very asymmetric fission). In parallel, we designed and implemented a new algorithm to simulate the real-time quantum-mechanical evolution of a fissioning nucleus through time-dependent DFT (TDDFT). For the first time, we obtained TDDFT estimates of the total kinetic energy (TKE) in the fission of ^{239}Pu for nearly all fragmentations and showed the impact of the energy functional on these estimates. Finally, we partnered with Petar Marevic at University of Zagreb to estimate the spin of all fission fragments in the fission of ^{239}Pu and ^{235}U using microscopic theory.

Mission Impact

A predictive theory of the fission process is essential to properly evaluate nuclear data and deliver reliable nuclear data libraries for end-user applications. Such libraries play an important role in enhancing the fundamental understanding of aging nuclear weapons systems or maintaining and enhancing the safety, security, and effectiveness of the U.S. nuclear weapons stockpile. They are also one of the most important diagnostic tools for Nuclear Forensics. Our work has improved the LLNL evaluation pipeline by delivering a new theoretical capability to perform fully quantum-mechanical simulations of fission dynamics. More broadly, we have developed new science and technology tools and capabilities to meet future national security challenges.

Publications

Marevic, Petar, Nicolas Schunck, and Marc Verriere, "Microscopic theory of angular momentum distributions across the full range of fission fragments." *Physical Review C*. (2025) [arXiv:2506.10777]. LLNL-JRNL-2007093. <https://doi.org/10.1103/yr2c-nvf3>

Bjelcic, Antonio, and Nicolas Schunck. 2025. "Computing the QRPA level density with the finite amplitude method." *Computer Physics Communications* 306, 109387 (2025).
<https://doi.org/10.1016/j.cpc.2024.109387>. LLNL-JRNL-866460.

Posters

Siwach, Pooja, Marc Verriere, and Nicolas Schunck. 2024. "Impact of quantum correlations on fission fragments." (Poster Presentation at 2024 SciDAC PI meeting, Washington, DC, July). LLNL-POST-866489.

Presentations

Pooja Siwach, Marc Verriere, Nicolas Schunck, 2024, "Impact on quantum collective correlations on fission fragment properties." (Presented at 2024 Fall Meeting of the APS Division of Nuclear Physics, Boston, MA, October 2024). LLNL-PRES-870350

Nicolas Schunck, Marc Verriere, Antonio Bjelcic, Pooja Siwach, Petar Marevic, 2024, "LLNL FPY Modeling and Evaluation." (Presented at CSWEG, Brookhaven National Laboratory, November 2024). LLNL-PRES-2011738.

Nicolas Schunck, 2024, "Microscopic theory of nuclear fission." (Presented at 5th Gogny Conference Nuclear Structure and Reactions, Paris, France, December 2024). LLNL-PRES-2002024.

Nicolas Schunck, 2025, "Using microscopic fission theory inputs to compute independent yields and the prompt fission spectrum." (Presented at Nuclear Data 2025, Madrid, Spain, June 2025). LLNL-CFPRES-2007296.

Siwach, Pooja, Nicolas Schunck, and Marc Verriere, "Impact on quantum collective correlations on fission fragment properties". 2024 Fall Meeting of the APS Division of Nuclear Physics, Oct. 6–10, 2024. LLNL-PRES-870350.

24-LW-043: Unraveling the Dynamics of Nucleosome Arrays: Identifying Key Factors that Modulate Gene Access

Project Overview

The organization of genomic DNA into chromatin is a fundamental determinant of genome stability, regulation, and cellular function. Nucleosomes, the basic repeating units of chromatin, assemble into higher-order structures whose organization and heterogeneity remain difficult to characterize using conventional ensemble-averaged techniques. A key need in the field is the development of experimental approaches capable of directly visualizing nucleosome assemblies and their structural variability at the single-molecule level.

This LDRD Lab-Wide project focused on establishing and evaluating atomic force microscopy (AFM)-based approaches for the characterization of nucleosome assemblies. The work emphasized experimental workflows for preparing, imaging, and assessing multi-nucleosome systems, rather than isolated single nucleosomes. Through method development and exploratory measurements, the project demonstrated the feasibility of applying scanning probe microscopy to investigate chromatin-relevant assemblies and provided preliminary insight into the strengths and limitations of this approach for future quantitative studies. Results and lessons learned from this effort were disseminated to the broader scientific community through multiple national conference presentations, helping to position LLNL for continued work in chromatin and genome organization research.

Mission Impact

This research contributed to LLNL missions by advancing experimental capabilities in high resolution imaging and biophysical characterization of complex biological systems. The development and evaluation of AFM-based workflows for nucleosome assemblies strengthened Laboratory expertise in scanning probe microscopy, supported cross-disciplinary collaboration between biosciences and materials science, and enhanced LLNL's visibility in the broader structural biology community. The outcomes of this work are relevant to DOE and NNSA missions that depend on a fundamental understanding of genome organization, biomolecular structure, and complex biological processes, and they provide a foundation for future programmatic research and external collaborations.

Publications, Presentations, and Patents

Wang, Y. 2024. Poster presentation. Biophysical Society Annual Meeting, Spring 2024.

Wang, Y. 2024. Poster presentation. FASEB Science Research Conference: Dynamic DNA Structures in Biology, 2024.

Wang, Y. 2025. Poster presentation. Society for Industrial Microbiology and Biotechnology (SIMB) Annual Meeting, 2025.

24-LW-045: A Multifunctional, Artificial Solid-Electrolyte Interface for Anode-Free Solid-State Batteries

Project Overview

New battery technologies that can store more energy, last longer, and be produced more sustainably than today's lithium-ion batteries are desperately needed. One of the most promising approaches is the development of anode-free solid-state batteries (AFSSBs), which could provide much higher energy density and improved safety. However, these batteries face a critical challenge: when lithium metal is deposited inside the battery during operation, it tends to grow unevenly. This instability shortens battery life and prevents AFSSBs technology from becoming commercially viable.

In this project, we explored new ways to make lithium deposit more evenly by combining two strategies. First, we developed a coating layer called an artificial solid electrolyte interphase (made of a polymer(s), Li-based inorganic salt, and additives) that helps lithium grow smoothly and prevents damaging reactions inside the battery. Second, we redesigned the structure of the current collector -the surface where lithium deposits- using advanced manufacturing techniques to create three-dimensional patterns that can accommodate changes during cycling. With this approach, we significantly improved battery performance, filed two patent applications, and began publishing results. We also started a collaboration to develop new machine learning methods to accelerate materials discovery, established collaborations with international research partners, and engaged in career development and outreach programs. Together, these results represent a major step toward making anode-free solid-state batteries practical, which could ultimately lead to safer, more powerful, and more sustainable energy storage systems for national energy security.

Mission Impact

This project directly advances Lawrence Livermore National Laboratory's mission in energy security by addressing one of the most pressing challenges in next-generation batteries: enabling safe, high-energy, and sustainable anode-free solid-state batteries. By developing new coatings and three-dimensional current collector designs, we created capabilities in polymer and inorganic salts engineering, additive manufacturing, and machine learning-guided experimentation that expand the Laboratory's core competencies in advanced materials and manufacturing and high-performance computing. The results position LLNL at the forefront of energy storage innovation and open new research directions in energy materials, electrochemistry, and autonomous discovery. The knowledge gained and intellectual property generated are highly relevant to the Department of Energy's efforts to accelerate energy technologies, to the National Nuclear Security Administration's interest in advanced materials and predictive modeling, and to other federal agencies focused national security.

Presentations

Erika P. Ramos, Nirmal A. Deshpande, Yuliang Zhang, Andre Fatehi, Giovanna Bucci. "Advancing Anode-Free Solid-State Batteries through 3D Current Collector Structuring and Polymer-Based Artificial SEI Engineering". Presented at European Conference on Solid State Chemistry (ECSSC), Spain, September 2025.

Erika P. Ramos, Nirmal A. Deshpande, Yuliang Zhang, Andre Fatehi, Metallic Nucleation Seeds Enable Uniform Lithium Deposition in Anode-Free Solid-State Batteries. ACS Meeting. USA. 2025.

Erika P. Ramos, Nirmal A. Deshpande, Yuliang Zhang. Korea Institute of Science and Technology and Lawrence Livermore National Laboratory workshop. USA, 2024.

Erika P. Ramos, Nirmal A. Deshpande, Yuliang Zhang. An Artificial Solid-Electrolyte Interphase for Anode-Free Solid-State Batteries. 24th International conference on solid state ionics. UK. 2024.

Patents

Ramos, Erika, et al. "Protective films and methods for using same." Patent application filed with IL, no. IL 33987-5. 2024.

Ramos, Erika, et al. "Methods for making and using current collectors." Provisional patent application no. 2025-018. 2025.

Other Outputs

Capstone project at California State University, Chico: "Battery Testing Automated Platform." Awarded 1st place, Most Outstanding Project, 2025.

The IL 33987-5 patent was selected for The Technology Innovation and Partnership Program, 2025.

Established a MTA with Dr. Pedro Aranguren at CIC energiGUNE. Currently preparing a manuscript that leverages our 3D-Ag CC invention with sulfide-based solid electrolytes (SEs).

Established a MTA with Dr. SeYoung Kim at KIST for Li metal anode protection using our ASEI invention. Currently, obtaining promising results with halide SEs.

24-LW-049: Understanding Rhenium-Isotope Behavior During the Rise of Earth's Atmospheric Oxygen

Project Overview

The rise of oxygen in Earth's atmosphere promoted the evolution of complex life, and understanding this history provides critical context for interpreting Earth system responses to environmental change. This project measured rhenium isotopes ($\delta^{187}\text{Re}$) in sedimentary samples spanning major oxygenation events to establish Re as a paleo-redox and weathering proxy. We analyzed geological samples spanning 2.4 billion years, weathering profiles through organic-rich shales, deep borehole samples revealing unexpected modern carbon in ancient rocks, and uranium ore concentrates for nuclear forensic applications. Results validated Re as a weathering proxy through coupled Re-organic carbon oxidation, revealed thermal and oxidative fractionation mechanisms, and demonstrated Re isotope potential for uranium source attribution. This work provides fundamental understanding of Re isotope systematics with implications for reconstructing Earth's atmospheric oxygen history and contributes to LLNL's nuclear forensics capabilities.

Mission Impact

This work addresses fundamental research gaps in utilizing Re isotopes as a weathering and paleo-redox proxy, with implications spanning geochemistry, and nuclear forensics. Improved understanding of Earth's oxygenation history and oxidative weathering processes directly informs carbon-climate feedbacks and how the Earth system responds to environmental perturbations. This work supports LLNL's Mission Focus Area in Earth System Resilience and complements Core Competencies in Earth & Atmospheric Science and Nuclear, Chemical, and Isotopic Science & Technology.

Critically, this project built fundamental capacity in Re isotope geochemistry and established novel applications to nuclear forensics through uranium ore concentrate analysis. The published work (Sullivan et al. 2024, EPSL; Grant et al. 2025, Chemical Geology) demonstrates LLNL's leadership in stable isotope geochemistry. This positions LLNL for potential NNSA nuclear forensic studies and DOE BER funding opportunities in Earth system science.

Publications

Ghazi, Layla, Katherine E. Grant, Anthony Chappaz, M. Danish, Bernhard Peucker-Ehrenbrink, and Julie C. Pett-Ridge. 2024. "The Global Biogeochemical Cycle of Rhenium." *Global Biogeochemical Cycles* 38: e2024GB008254. <https://doi.org/10.1029/2024GB008254>. LLNL-JRNL-868303.

Grant, Katherine E., Mathieu Dellinger, Alexander J. Dickson, Mateja Ogric, Kate Horan, Steven Petsch, and Robert G. Hilton. 2025. "Validating the Rhenium Proxy for Rock Organic Carbon Oxidation Using Weathering Profiles." *Chemical Geology* 671: 122464. <https://doi.org/10.1016/j.chemgeo.2024.122464>. LLNL-JRNL-2000144.

Sullivan, Daniel L., Gregory A. Brennecka, Katherine E. Grant, and Ariel D. Anbar. 2024. "Rhenium Isotope Reconnaissance of Uranium Ore Concentrates." *Earth and Planetary Science Letters* 644: 118898. <https://doi.org/10.1016/j.epsl.2024.118898>. LLNL-JRNL-[add number].

Conference Presentations

Grant, Katherine E., Robert G. Hilton, Susan L. Brantley, Nicole M. Fernandez, Patrick Fulton, and Valier V. Galy. "Why Is There Young Carbon in Deep Geologic Boreholes? A Combined Approach Using Carbon Isotopes and Thermal Analysis." Poster presented at Goldschmidt Conference, Chicago, IL, August 2024. LLNL-POST-868483.

Grant, Katherine E. "Using Rhenium, $\delta^{187}\text{Re}$, and RPO- ^{14}C to Trace the Fate of Rock Organic Carbon in the Critical Zone." Invited seminar presented at Oxford University, Oxford, UK, April 18, 2024.

Sullivan, Daniel L., Gregory A. Brennecka, Katherine E. Grant (presenting author), and Ariel D. Anbar. "Rhenium Isotope Reconnaissance of Uranium Ore Concentrates." Poster presented at Goldschmidt Conference, Lyon, France, July 2023.

24-LW-053: Data-Driven Constraints on Soil-Carbon Persistence in Earth-System Models

Project Overview

Uncertainties in soil organic carbon (SOC) persistence represent a major challenge with Earth system models (ESMs) varying by up to 200 Pg C in their predictions. This project developed novel data-driven constraints to benchmark soil carbon persistence in ESMs. We directly quantified petrogenic organic carbon (OC_{petro}) contributions in soils across the continental United States using ramped pyrolysis/oxidation analysis of NEON network samples, revealing that OC_{petro} can bias soil carbon age estimates by hundreds of years. We created machine learning-derived global predictions of soil radiocarbon with rigorous uncertainty quantification and developed a generalizable framework for benchmarking soil carbon ages across CMIP6 ESMs.

Mission Impact

This LDRD project addresses fundamental research gaps in estimating soil carbon persistence globally and benchmarking soil carbon ages in ESMs. Improved estimates of soil carbon persistence are critical for understanding carbon sequestration potential. This work directly supports LLNL's Mission Focus Area in Earth System Resilience and complements Core Competencies in Earth & Atmospheric Science and Nuclear, Chemical, and Isotopic Science & Technology.

Critically, this LDRD built key capacity in soil carbon cycle modeling within a niche not yet covered by other National Labs, positioning LLNL to participate in major DOE funding opportunities on ESM development and analysis through programs like ILAMB (International Land Model Benchmarking) and AI4ESP (Artificial Intelligence for Earth System Predictability).

Publications

Fromm, S. von, A. Hoyt, C. Sierra, K. Georgiou, S. Doetterl, and S. Trumbore. 2024. "Controls and relationships of soil organic carbon abundance and persistence vary across pedo-climatic regions." *Global Change Biology* 30, , no. 5 : 1-18. LLNL-JRNL-860327.

Georgiou, K., C. Koven, W. Wieder, M. Hartman, W. Riley, J. Pett-Ridge, N. Bouskill, R. Abramoff, E. Slessarev, A. Ahlstrom, W. Parton, A. Pellegrini, D. Pierson, B. Sulman, Q. Zhu, and R. Jackson. 2024. "Emergent temperature sensitivity of soil organic carbon driven by mineral associations." *Nature Geoscience* 17, , : 205-212. LLNL-JRNL-844927.

Posters

Grant, Katherine, Katerina Georgiou, and Karis McFarlane. "Rock derived carbon contributes radiocarbon-free organic carbon to soils across the continental USA." (Poster Presentation at American Geophysical Union, Washington DC, December 2024. LLNL-POST-871661.

Presentations

Katerina Georgiou. "Global distribution and temperature sensitivity of mineral-associated soil organic carbon." (Presented at Soil Organic Matter Symposium, Morocco, May 2024).

Katerina Georgiou. "Looking under the hood: soil carbon pool distributions and benchmarks for Earth system models." (Presented at 7th Training Course in Land Carbon Cycle Modeling, Virtual (Cornell University), June 2024).

Katherine Grant. "How much of the soil carbon reservoir is rock-derived? A perspective using a soil radiocarbon database and thermal analysis." (Presented at American Geophysical Union Fall Meeting, San Francisco, CA, December 2023).

Katherine Grant. "Organic carbon preservation across scales; how rock derived organic carbon influences the modern carbon cycle." (Presented at University of Pittsburgh Department of Geology & Environmental Science Colloquium, University of Pittsburgh, October 2025).

Katherine Grant, Katerina Georgiou, Karis McFarlane. "Rock derived carbon contributes radiocarbon-free organic carbon to soils across the continental USA." (Presented at International Radiocarbon Meeting, Krakow Poland, June 2025).

24-LW-059: Microwave Volumetric Additive Manufacturing for Ceramics

Project Overview

Current advanced manufacturing methods for ceramics are limited to layer-by-layer construction that is time consuming. Recent development of an optical volumetric additive manufacturing (VAM) technology has enabled rapid 3D printing in a singular step. However, optical VAM is limited to transparent photo resins. Here we develop a scalable one-of-a-kind microwave VAM (M-VAM) system for ceramic materials. The concept relies on utilizing a high-power antenna array coupled to a beamforming algorithm to superimpose multiple microwave beams and deliver localized energy to arbitrary 3-D volumes. In this research, we have (1) synthesized a microwave sensitive ceramic feedstock with high solid ceramic loading volumes (up to 60%), (2) developed a multi-physics model that effectively integrates the thermal diffusion effects of microwaves with the chemical kinetics of ceramic binding to predict cured shapes and times and optimize process parameters and (3) built a near-field microwave beamforming hardware system that can focus energy and cure a mm-sized region in the feedstock.

Mission Impact

This project supported the Manufacturing process development priority of the Accelerated Materials and Manufacturing Initiative and Core Competency by developing an advanced manufacturing (AM) method for volumetric printing of optically opaque polymer materials, relevant towards emerging fields such as flexible electronics and composites. This research led to institutional capabilities of a new AM technology, well-aligned with different technology tracks of the Advanced Manufacturing laboratory.

Publications, Presentations, and Patents

Mukherjee, S., Et al., 2024. Towards microwave VAM: generation of a computational multi-physics model for localized curing. *Additive Manufacturing Letters*, 10, p.100209.

Schwartz, J.J., Mukherjee, S. and Baluyot, E.V., 2024. Systems and methods for microwave additive manufacturing. U.S. Patent Application 18/075,947.

Mukherjee, S., Et al., Focused Towards Microwave VAM: Rapid Curing of Ceramic Binder Mixtures using Microwave Radiation, 2024 Solid Freeform Fabrication Symposium.

Rosenberg E. Et al., Multiphysics Material Screening for Microwave Volumetric Additive Manufacturing, 2024 MRS Fall Meeting & Exhibit.

Vandenbrande J. Et al., Microwave Radiation in Volumetric Additive Manufacturing to create 3D Ceramics, 2024 MRS Fall Meeting & Exhibit., 2024 MRS Fall Meeting & Exhibit.

James Kelly Et al., Rapid printing of 3-D ceramic materials using microwave volumetric additive manufacturing, International Conference and Expo Advanced Ceramics and Composites 2025.

<https://www.llnl.gov/article/51756/llnl-looks-revolutionize-3d-printing-through-microwave-technology>

IPO-LLNL-M-VAM

24-LW-060: Produce and Power: Assessing the Effects of Agrivoltaics on the Food–Water–Energy Nexus

Project Overview

The growing demand for energy in the US has intensified competition for land between solar energy development and agriculture. Agrivoltaics—the co-location of solar panels with crops or livestock—offers a potential solution that allows land to serve both energy and agricultural needs, with potentially co-benefits for both industries. However, limited data exist on where agrivoltaic systems are most feasible and how they influence environmental and agricultural outcomes. This research sought to identify optimal locations for agrivoltaic development across the United States and to evaluate their environmental and agronomic impacts in a field setting.

In the first year, we conducted a nationwide assessment that integrated environmental, economic, and policy data to evaluate agrivoltaic potential at the county level. Factors such as water availability, agricultural productivity, farm income, and energy infrastructure were analyzed to develop an opportunity index for agrivoltaics. We also conducted a public sentiment analysis of news media coverage to assess how perspectives on agrivoltaics vary across states, since public pushback and restrictive local policies indirectly developed due to this pushback can waste valuable development resources. We compiled all of this geospatial data together to yield a high-resolution land assessment of the United States and where agrivoltaics may be most advantageous to be proposed for development.

In the second year, we performed field experiments in Mililani, Hawaii, in collaboration with the Hawaii Agricultural Research Center and the University of Hawaii at Manoa. The study measured gas emissions from soil, soil moisture, and crop yield in jalapeno pepper plots grown under solar panels and in adjacent full-sun control plots. We found that gas emissions from soils under panels were approximately half those of the control plots, marking the first quantification of such emissions in an agrivoltaic setting. Soil moisture patterns were more complex than expected, and crop yields under the panels were about 50 percent lower and ripened roughly two months later. These results demonstrate that agrivoltaics can provide measurable environmental benefits but may involve trade-offs in crop performance, informing future system designs that optimize both energy and agricultural productivity.

Mission Impact

This research advances Lawrence Livermore National Laboratory’s mission to enhance national energy security, environmental stewardship, and resilience by developing science-based solutions for locally produced energy systems. The agrivoltaics project strengthened LLNL’s capabilities in coupled energy–agriculture–environmental systems modeling and field-based measurement of soil gas emission dynamics, establishing new expertise in land-use efficiency and energy integration. Conducted in Hawaii—a location of critical strategic importance for U.S. military operations, yet almost entirely dependent on imported oil from nations such as Libya, Indonesia, and Argentina – this work directly supports the Department of Energy (DOE) and National Nuclear Security Administration (NNSA) priorities to improve energy reliability and resilience for isolated and defense-relevant regions. By exploring how solar energy can coexist with agricultural production,

the project contributes to reducing Hawaii's dependence on foreign fuels, improving long-term energy affordability, and informing pathways for energy independence. The research also aligns with the missions of other federal agencies, including the U.S. Department of Agriculture and the Department of the Interior, by providing data-driven insights for smart agriculture and sustainable energy development.

Publications

Donnison, Caspar L., Alexander Stanley, Whitney Kirkendell, Tao Dai, and Kimberley Mayfield. "Where Agrivoltaics Work: Public Sentiment and Co-benefits Across the U.S." Submitted to Nature Communications, October 20, 2025. LLNL Technical Report RR: LLNL-TR-2011216. Lawrence Livermore National Laboratory, 2024.

Presentations and Awards

Donnison, Caspar L. "Agriculture and Solar Power: An Unlikely Alliance." Presented at the LLNL Research Slam, Livermore, California, September 25, 2024. (Third Place Award)

Donnison, Caspar L. "Agriculture and Solar Power: An Unlikely Alliance." Presented at the Bay Area Research Slam (BARS), San Francisco, California, October 3, 2024. (Third Place Award)

24-LW-062: Forging New Pathways to Improved Nuclear-Reaction Predictions

Project Overview

We proposed to improve nuclear-reaction predictions to provide a better link between scattering experiments and nuclear structure. This link is particularly needed to understand complicated structure features that emerge in nuclei far from stability. Building upon state-of-the-art ingredients, we developed a new capability to accurately include modern nucleon-nucleon interactions in proton-induced knockout reactions. The tools developed in this project position us to include effects of the target medium in nucleon-induced knockout reactions. These improvements to nuclear-reaction descriptions help to harness the wealth of experimental data produced by the DOE-funded FRIB on nuclei approaching the limits of stability, bringing the community closer to unravelling the mystery of how protons and neutrons arrange themselves inside the nucleus.

Mission Impact

This project has laid the foundation toward better reaction predictions which launch LLNL further into the forefront of probing new physics in exotic nuclei. This project supports LLNL's Stockpile Stewardship mission through better reaction calculations. Improved reaction descriptions greatly enhance the scientific community's ability to extract structure information from the wealth of reaction data coming from FRIB. This helps to strengthen the already-healthy relationship between LLNL and FRIB. Additionally, we further cultivated collaborations with Washington University in St. Louis and the University of Osaka which expands LLNL's scientific network.

Publications

Atkinson, Mack, and Wim Dickhoff. 2024. "Neutron skins: A perspective from dispersive optical models." *Frontiers in Physics* 12, , no. 1487314. <https://doi.org/10.3389/fphy.2024.1487314>. LLNL-JRNL-868759.

Atkinson, Mack, and Willem Dickhoff. 2025. "Learning from knockout reactions using a dispersive optical model." *Frontiers in Physics* 12, , no. 1505982. <https://doi.org/10.3389/fphy.2024.1505982>. LLNL-JRNL-870309.

Presentations

Mack Atkinson, 2024, "Nucleus-Informed NN Interaction from a Dispersive Optical Model." (Presented at Towards a consistent approach for nuclear structure and reactions: microscopic optical potentials, Trento, Italy, June 2024).

Mack Atkinson, 2024, "A consistent treatment of bound and scattering states through the dispersive optical model." (Presented at Theory Seminar, CEA, Bruyeres-le-Chatel, France, December 2024).

Mack Atkinson, 2025, "A consistent treatment of bound and scattering states through the dispersive optical model." (Presented at Theory Seminar, Osaka University, February 2025).

Mack Atkinson, 2024, "Consistently treating bound and scattering states in many-body methods." (Presented at Fifth Gogny Conference, Paris, France, December 2024).

Mack Atkinson, 2025, "Nucleus-Informed Nucleon-Nucleon Interaction from a Dispersive Optical Model." (Presented at APS April Meeting 2025, Anaheim, CA, March 2025).

24-LW-066: Self-Assembled Molecular Containers as Artificial Water Channels: Towards Biomimetic Desalination Membranes

Project Overview

Global water scarcity demands advances in desalination technologies that can deliver more fresh water with less energy. Current reverse osmosis membranes are fundamentally limited by a trade-off between how much water they can pass and how well they block salts. To address this challenge, we developed a bottom-up strategy to design and test artificial water channels that mimic the efficiency of biological proteins but are built from robust synthetic molecules.

Over two years, we synthesized and evaluated more than twenty molecular channel candidates, including supramolecular macrocycles and nanographene pores with atomically precise structures. We showed that small chemical modifications allow direct control over pore size and chemistry, which in turn govern water permeability and salt rejection. In collaboration with university partners, we reported the first experimental demonstration of water transport through a nanographene pore, bridging a long-standing gap between simulation and experiment. Several of the artificial channels we developed achieved water–salt selectivity beyond conventional polymer membranes, highlighting their potential for next-generation desalination and precision separations.

Mission Impact

Our project directly addressed Lawrence Livermore National Laboratory's (LLNL) mission area in Energy Security by advancing materials that can transform water treatment efficiency and resilience. The ability to design, synthesize, and test artificial channels with angstrom-level precision enhances LLNL's capabilities in supramolecular chemistry, nanofluidics, and membrane science, creating a foundation for new collaborations and external funding opportunities. The results are highly relevant to DOE and NNSA missions in sustainable desalination, isotope enrichment, and critical material recovery, while also supporting broader federal priorities in environmental security and energy resilience.

Publications, Presentations, and Patents

Yuhao Li, Mamun Sarker, Alexander Sinitskii, and Aleksandr Noy. 2025. "Water permeation observed in stacked nanographene with an [18]annulene pore." (Poster Presentation at 19th International Symposium on Macrocyclic and Supramolecular Chemistry, Kyoto/Japan, May). LLNL-POST-2006116.

Yuhao Li, 2024, "Engineering Tunable Macrocyclic Subnanometer Pores as Biomimetic Channels for Ångstrom-Precision Separation." (Presented at 2024 MRS Spring Meeting & Exhibit, Seattle, Washington, April 2024).

24-LW-069: Volumetric Subtractive Manufacturing

Project Overview

Manufacturing small negative features has been extremely challenging in the field of whole additive manufacturing (AM). Due to overcuring, diffusion and refractive index increase, the achievable smallest negative feature and fidelity is always worse than the smallest positive one using AM methods. Additionally, attempting to print multi-scale feature sizes in the same exposure has proven to be challenging in digital light processing (DLP) printing due to diffusion and inhibition. To address these challenges, we have developed a hybrid additive and subtractive manufacturing approach on a DLP platform with a dual-wavelength photopolymers to be able to print multi-scale features and small negative features with accuracy. We have demonstrated a first-of-its-kind Volumetric Subtractive Manufacturing by fabricating non-planar double helix fluidics with photo-degrading polymers. This work has the potential to shift the paradigm of DLP AM techniques by incorporating subtractive manufacturing as a new degree of freedom for enhancing the achievable print resolution and enabling corrective and adaptive manufacturing.

Mission Impact

The techniques developed in this project enable us to fabricate complex objects with two complementary tools: print positive features by photo-polymerization and print negative features by photo-degradation. It also allows us to fabricate structures in a top-down approach: carving materials with light into the desired geometry by photo-degradation. Moreover, this will make on-machine characterization, qualification and correction readily achievable when equipped with real-time monitoring, which will improve the part accuracy and reproductivity, and reach the goal of 'born certified'. This project advances our Advanced Materials and Manufacturing Core Competency and general Manufacturing Complex in DOE and NNSA. The new techniques and capabilities developed in this project will enable NNSA to create new ways of responding to and solving national security challenges.

Publications

Howard, Holden, Benjamin Alameda, Martin De Beer, Magi Mettry-Yassa, Johanna Schwartz, and Dongping Terrel-Perez. 2025. "Hybrid Additive and Subtractive Manufacturing of Dual-Wavelength Photopolymer Thermosets." *Advanced Materials Technologies*, (September).<https://doi.org/10.1002/admt.202500997>. LLNL-JRNL-2004128.

Posters

Howard, Holden, Benjamin Alameda, Magi Yassa, Martin De Beer, Johanna Schwartz, and Dongping Terrel-Perez. 2024. "Photo-selective Polymer Thermosets for Hybrid Additive and Subtractive Manufacturing." (Poster Presentation at Additive Manufacturing of Soft Materials Gordon Research Conference, Smithfield, Rhode Island, United States, August). LLNL-POST-867592.

Presentations

Holden Howard, Dongping Terrel-Perez, Benjamin Alameda, Martin De Beer, Magi Yassa, Isabel Arias Ponce, Johanna Schwartz, 2025, "Hybrid Additive and Subtractive Manufacturing of Wavelength-Selective Cleavable Polymer Thermosets." (Presented at ACS Spring, San Diego, California, US, March 2025).

Patents

Alameda, Benjamin, Magi Yassa, Martin De Beer, Holden Howard, Dongping Terrel-Perez, Johanna Schwartz, Isabel Arias Ponce, and Ishan Joshipura. "Polymers with photoselective polymerization and degradation pathways." Patent application number: 63/656,502.

Terrel-Perez Dongping, Mettry-Yassa Magi, De Beer Martin, Shusteff Maxim, Huang Sijia, Alameda Benjamin, Fong Erika, Schwartz Johanna. "Systems and methods for volumetric subtractive manufacturing and hybrid volumetric additive/subtractive manufacturing." Patent application number: 18/978,297.

24-LW-070: De Novo Synthesis and Near-Atomic-Resolution Imaging of Host Immune Receptors Critical for Pathogen Recognition

Project Overview

The innate immune system serves as the body's first line of defense against invading pathogens, responding rapidly through the deployment of immune cells at common sites of infection, such as the skin and airways. These immune-cell sentinels express a range of highly conserved receptors, including Toll-like receptors (TLRs), which recognize and bind to pathogen-derived components. This recognition event triggers intracellular signaling cascades that initiate and coordinate immune responses. Despite their significance, the complete structural characterization of full-length TLRs, including their extracellular domain (ECD), transmembrane domain (TMD), and Toll/interleukin-1 receptor (TIR) domain, remains incomplete.

In this study, we examined the expression and isolation of human TLR4 incorporated into nanodiscs using two approaches: a cell-free synthesis system and a cell-based transfection strategy employing Expi293F cells derived from the human embryonic kidney lineage. Our findings demonstrate that NLP-bound human TLR4 produced via the cell-based method yielded functional protein suitable for time-resolved single-particle cryo-electron microscopy (cryo-EM). This advancement enables structural characterization of full-length TLR4, maintaining the integrity of its extracellular domain, transmembrane domain, and Toll/Interleukin-1 receptor (TIR) domain.

High-resolution reconstruction of sensitive proteins such as TLR4 requires vitrified grids with uniform ice thickness to optimize contrast transfer function and minimize artifacts caused by the air-water interface, which can lead to protein denaturation and unfolding. Meeting this challenge required not only a new approach to sample preparation but also the resolution of key engineering barriers in device fabrication. Specifically, we achieved precise control of nanofluidic channel dimensions to reliably handle picoliter-scale volumes, and for the first time etched large, free-standing, ultra-thin electron-transparent silicon nitride films that serve as the imaging window. Building on these innovations, we developed a nanofluidic electron microscopy (nanoEM) chip and validated its performance using apoferritin. This platform enables reproducible, high-throughput preparation of vitrified samples with improved reliability, establishing a robust foundation for structural studies of complex membrane proteins.

Mission Impact

A fuller understanding of the structural mechanism of signal transduction of full length TLRs are entirely novel and have large implications for our understanding of innate immune response. This mechanistic characterization of the TLR4 pathway is transferrable to high-throughput diagnostic and therapeutic platforms. The novel sample environment platform developed in this project is applicable to other structural studies using cryo-EM. This study bolsters LLNL's biotechnology Core Competencies in cell- and cell-free based membrane protein production, functional characterization, and structural biology. The results and technology developed are directly relevant to the mission

space within DOD, DOE, DHS, NIH and NASA, where membrane bound receptor networks play a critical role in pathogen sensing and detection.

Publications, Presentations, and Patents

Abisoye-Ogunniyan*, A., Nikfarjam, S., Laurence, A. M., Shelby, M. L., Frank, M., Coleman, M., Rasley, A., Narayanasamy, S. R. *. Expression and Isolation of Full-length Human TLR4 in Nanolipoprotein Particles for Structural Analysis via cryo-electron microscopy, *Immunology 2025*-The Annual Meeting of the American Association of Immunologists, 2025. LLNL-ABS-2001103.

TLR4- Expression and Characterization of a complex membrane protein. Laurence, A., Nikfarjam, S., Abisoye-Ogunniyan, A., Narayanasamy, S.R., Shelby, M.L., Frank, M., Coleman, M. Expression and Isolation of Full-Length Human TLR4 in Nanolipoprotein Particles for Future Structural Analysis via Cryo-EM, 2025. LLNL-POST-2000294.

24-LW-076: Beyond Biomass-based Carbon Removal and Sequestration: A Comprehensive Greenhouse Gas Assessment of Biomass-Based Carbon Dioxide Removal and Sequestration

Project Overview

Biomass-based Carbon Removal and Storage (BiCRS) is a suite of technological pathways that provide a relatively affordable and high-potential way to remove carbon dioxide from the atmosphere and simultaneously re-purpose residual biomass. BiCRS technologies are individually optimized to different biomass feedstocks, temperatures and oxygen, with the primary goal of capturing a high percentage of biomass-derived carbon dioxide and storing it in permanent below-ground storage (i.e. geologic storage), and a secondary goal of producing renewable energy. The current standard for BiCRS life cycle assessments does not account for carbon dioxide, methane and nitrous oxide fluxes from surface soil amendment of BiCRS byproducts (e.g. char, ash) and their alternate fates. This is partly due to a paucity of empirical data due to the novelty of BiCRS conversion technologies, the range in feedstocks, and the heterogeneity of soils to which they might be amended. To fill this gap in the life-cycle assessment and provide a realistic range of parameters for a soil amendment component of the BiCRS life cycle assessment, we conducted an incubation experiment to measure soil carbon changes, microbial respiration, methane fluxes, and nitrous oxide fluxes from two different soils amended with char- and ash- byproducts from biomass after gasification to hydrogen, fast pyrolysis to bio-oil, and torrefaction.

Our results suggest that nitrous oxide and methane emission or consumption from BiCRS char amendments to soil are context dependent. Nitrous oxide emissions from amendments are higher in soils with higher pH, whereas some char amendments to low pH soil can reduce N₂O emissions relative to control. In contrast, methane is emitted from BiCRS char amended to low pH soil, but consumed or neutral relative to control when amended to high pH soil. We present carbon and nitrogen mass balance throughout the experiment to help understand short-term durability of BiCRS chars and their counterfactuals, and preliminary suggestions for revisions to the broader BiCRS Measurement, Reporting, and Verification framework.

Mission Impact

This study supports the LLNL Mission of Energy Security within the Focus Area in Earth System Resilience by contributing to both renewable energy sources and carbon dioxide removal efforts. We created a new cross-division partnership between Nuclear And Chemical Science and Computational Engineering divisions and a new collaboration with the National Lab of the Rockies, who provided byproduct material for the incubation experiment and continue to collaborate with us on a parallel study of the biogeochemistry of BiCRS bioproducts. The results of this project are being integrated into Measurement, Reporting, and Verification frameworks commissioned by the Department of Energy, to improve the actual net carbon removal calculations for BiCRS pathways throughout their entire life cycle.

Publications, Presentations, and Patents

Mayer, Allegra, Aaron Chew, Alvina Aui, Jennifer Pett-Ridge. 2024. “Beyond BiCRS: A Comprehensive Greenhouse Gas Assessment of Biomass-Based Carbon Dioxide Removal and Storage.” *American Geophysical Union Fall Meeting*. Oral Presentation.

Mayer, Allegra, Aaron Chew, Alvina Aui, Jennifer Pett-Ridge. 2025. “Beyond BiCRS: A Comprehensive Greenhouse Gas Assessment of Biomass-Based Carbon Dioxide Removal and Storage.” *University of California Merced Soil Carbon Biogeochemistry Groups*. Invited Seminar.

Mayer, Allegra, Aaron Chew, Alvina Aui, Jennifer Pett-Ridge. 2025. “A Comprehensive Greenhouse Gas Assessment of Biomass-Based Carbon Dioxide Removal and Storage.” *American Geophysical Union Fall Meeting*. Poster Presentation.

Mayer, Allegra, Aaron Chew, Alvina Aui, Wenqin Li, Jennifer Pett-Ridge. In Preparation. “A Comprehensive Greenhouse Gas Assessment of Biomass-Based Carbon Dioxide Removal and Storage.” *Environmental Science & Technology*.

24-LW-082: Algae-Cement Interactions as a Carbon-Negative Technology: Understanding Carbon-Dioxide Drawdown Potential as a Function of Water Chemistry Changes and Algal Growth

Project Overview

This project was motivated by the need to cultivate algae more reliably and at lower cost for the generation of bioproducts. A key challenge in large-scale algal production is the expense, steady supply, and emissions profile of nutrients, especially silicon and trace metals for diatoms, along with sufficient carbon dioxide. We explored whether waste cement, used in the form of mortar, could be repurposed as a low-cost additive that provides essential nutrients and improves the availability of dissolved carbon dioxide, thereby increasing algal growth and carbon capture.

We prepared and tested mortar at different concentrations and grain sizes and measured algal cell numbers, cell size, and carbon uptake. We also assessed alkalinity, analyzed metal release and assimilation, and examined nanoscale algal interactions with mortar fragments. Mortar concentrations between 0.1 and 0.3% (weight/volume) supported the strongest growth across a range of grain sizes. The likely explanation is a combination of fast release of beneficial substances from small grains and sustained release from larger grains over the course of the algal growth cycle. Cultures grown with mortar became more numerous, had larger cells, and assimilated more carbon dioxide than controls without mortar. Metals released from mortar and taken up by algae included iron, aluminum, manganese, zinc, vanadium, titanium, and silicon. Alkalinity increased significantly, consistent with the release of carbonates and the hydration of calcium oxide and magnesium oxide to form hydroxides in water. The higher alkalinity plausibly contributed to increased carbon uptake. Together, these results establish multiple mechanisms by which mortar additions can increase algal growth and yield, and they provide fundamental data on algal–cement interactions that can inform strategies for scale-up and potential carbon-negative applications.

Mission Impact

This work advances Lawrence Livermore National Laboratory missions by demonstrating a practical pathway to valorize an abundant industrial waste while improving biological carbon capture. It supports Department of Energy and National Nuclear Security Administration priorities in carbon management, environmental stewardship, and circular economy solutions. The project integrates and strengthens Laboratory capabilities in microanalysis and imaging with biological cultivation, enabling new single-cell and geochemical perspectives on carbon fixation. The results open new research directions at the interface of materials science and bioenergy, including optimization of mineral dosing and particle size distributions, evaluation of cement reuse after algal interaction, and techno-economic assessments of nutrient cost offsets. These directions can catalyze collaborations with cement recyclers and algal bioproduct companies and create opportunities for future staffing and partnerships.

Publications, Presentations, and Patents

Samo, Ty, Kristina Rolison, Jiaqi Li, John Rolison, Rhona Stuart, Keith Morrison, Xavier Mayali. Algae-cement systems as carbon negative technologies. 2023. Record of Invention.

Scott, Savannah, Kristina Rolison, and Ty Samo. 2024. "Optimizing Algal Cultivation: Evaluating Mortar as a Growth Additive for the Diatom *Phaeodactylum tricornutum*." Poster presented at the Summer Student Poster Symposium, Lawrence Livermore National Laboratory, Livermore, California, August 1.

Samo, Ty, Kristina Rolison, Jiaqi Li, John Rolison, Rhona Stuart, Keith Morrison, Xavier Mayali, and Peter Weber. 2025. "Diatom Growth, Biomass, and Carbon Fixation Is Enhanced When Cultivated with Aged Cement." Oral presentation at the International Conference on Algal Biomass, Biofuels and Bioproducts, Phoenix, Arizona, June 15 to 18.

23-SI-002: Advanced Energy-Storage Technologies for Extreme Conditions

Project Overview

Advanced Energy Storage for Extreme Conditions (AESTEC) developed a new capability for designing and fabricating energy storage devices that function in extreme conditions detrimental to conventional devices (e.g. temperature, mechanical stress, etc.). This project established an institution-level framework for the multiscale design and optimization of energy storage devices by unlocking critical scientific insights in ion transport, morphologic evolution, and solid mechanic under extreme conditions. We strategically leveraged LLNL's expertise in multiscale modeling, advanced materials and characterization, and design optimization to demonstrate the scope and impact of this powerful toolset in the area of energy storage. The culmination of this integration of multiscale modeling, advanced materials and characterization, and design optimization produced energy storage devices with exceptional performance under extreme conditions and critical insights into energy storage processes that are applicable to the nation's broader energy storage challenges.

Key outcomes of the project include:

1. Enabled the necessary infrastructure, tools, and understanding to produce a battery capable of retaining 50% of its energy density at -40°C
2. Developed new materials solutions for optimizing ion transport, phase evolution, and mechanics through coupled multiscale modeling and experiments (DIW and PuSL carbons, MnO_2 , and electrolytes)
3. Combined device simulation and optimization tools (e.g. LIDO/SMITH) into a novel framework to design coupled electrochemical systems for optimized environments
4. Trained the next generation of LLNL workforce in extreme-condition energy storage for diverse mission needs (>20 personnel)

Energy storage devices operate optimally in a relatively small range of environmental (e.g. temperature) and utilization (e.g. charge/discharge rate) conditions. When placed in conditions outside of this specified range, device performance can degrade by as much as 90% and catastrophic failure can occur. Furthermore, even under the optimal environmental and utilization conditions, current state-of-the-art devices require radical advances in energy storage technology to meet target goals set by the Department of Energy's Energy Storage Grand Challenge Roadmap. Both of these challenges boil down to a fundamental lack of mechanistic understanding about the key phenomena that degrade device performance, namely ion transport, morphological evolution, and solid mechanics. Acquiring a detailed understanding of these three phenomena and their relationships with each other will open up a path to designing energy storage devices that are tailor-made to function under a wide set of environments and use cases.

One of the major outcomes from this work was the confirmation that advanced materials and better designed devices improve energy storage device performance. Although this research is promising,

due to limited scope, the impact was provincial. This project strategically developed and leveraged these capabilities to demonstrate the full scope and impact of this powerful toolset. First, understanding of the key phenomena at the atomistic and mesoscale was accomplished via tight coupling of simulations and characterization of energy storage materials under extreme conditions. Here, the physics and mechanisms of dendrite nucleation and growth, ion intercalation, and bond strength were clarified and refined. This knowledge was then incorporated into device-level models and optimization tools coupled with additive manufacturing and device-level characterization providing insight into macro scale phenomena, like ion diffusion, dendrite formation and growth, and microcracking in electrodes.

Mission Impact

Advanced Energy Storage for Extreme Conditions (AESTEC) provides the institution level framework needed to position LLNL as a key contributor to the energy storage needs in extreme conditions particularly relevant to our nation's energy security and defense. The specific conditions of interest are extreme temperature, mechanical stress, and aging/lifetime concerns which are encountered in space, energy infrastructure, and weapons applications. By strategically enhancing LLNL's energy storage research efforts in modeling, optimization, materials, characterization, and additive manufacturing, the Laboratory can now make faster progress and more significant impacts to address these challenge areas. AESTEC has facilitated more seamless transfer of relevant knowledge and discoveries between the various energy storage technologies including origins of slow ion transport and sluggish kinetics, improved ink formulation, multiscale modeling integration, prototyping, and optimization algorithm. As such, AESTEC has impacted unique energy storage challenges that are relevant to LLNL's program needs and leverages the Laboratory's strengths and expertise in growth areas like space, infrastructure, and weapons. Notably, the incredibly important nature of these unique applications positions LLNL as complementary to existing energy storage research efforts from other organizations and has increased LLNL's footprint in this field due to the broader impact of the scientific challenges it addresses.

Publications

Lin, Dun, Swetha Chandrasekaran, Jean-Baptiste Forien, Xinzhe Xue, Anica Pinongcos, Emma Coester, Marcus A Worsley, and Yat Li. 2023. "3D-Printed Graded Electrode with Ultrahigh MnO₂ Loading for Non-Aqueous Electrochemical Energy Storage." *Advanced Energy Materials* 13, , no. 20 : 2300408. LLNL-JRNL-845347.

Chandrasekaran, Swetha, Dun Lin, Yat Li, and Marcus A Worsley. 2023. "Aerogels, additive manufacturing, and energy storage." *Joule* 7, , no. 5 : 866–883. LLNL-JRNL-855381.

Batista, Mariana Desireé Reale, Swetha Chandrasekaran, Bryan D Moran, Miguel Salazar de Troya, Anica Pinongcos, Zhen Wang, Ryan Hensleigh, Adam Carleton, Manhao Zeng, Thomas Roy, and others . 2023. "Design and additive manufacturing of optimized electrodes for energy storage applications." *Carbon* 205, , : 262–269. LLNL-JRNL-838972.

- Zhu, Cheng, Noah B Schorr, Zhen Qi, Bryan R Wygant, Damon E Turney, Gautam G Yadav, Marcus A Worsley, Eric B Duoss, Sanjoy Banerjee, Erik D Spoerke, and others . 2023. "Direct ink writing of 3D Zn structures as high-capacity anodes for rechargeable alkaline batteries." *Small Structures* 4, , no. 4 : 2200323. LLNL-JRNL-835018.
- Sun, Wenyu, Christine A Orme, Marcus A Worsley, and Liwen F Wan. 2024. "First-principles evaluation of MnO₂ polymorphs as cathode material in lithium-ion batteries." *Sustainable Energy & Fuels* 8, , no. 12 : 2718–2729. LLNL-JRNL-860544.
- Pinongcos, Anica B, Xinzhe Xue, Swetha Chandrasekaran, Marcus A Worsley, and Yat Li. 2025. "Innovative Electrode Design for Low-Temperature Electrochemical Energy Storage: A Mini Review." *Energy & Fuels* 39, , no. 13 : 6078–6096. LLNL-JRNL-870546.
- Xue, Xinzhe, Zhen Liu, Swetha Chandrasekaran, Samuel Eisenberg, Curtis Althaus, Megan C Freyman, Anica Pinongcos, Qiu Ren, Logan Valdovinos, Cathleen Hsieh, and others . 2025. "Interface-Controlled Redox Chemistry in Aqueous Mn₂/MnO Batteries." *Advanced Materials*, : 2419505. LLNL-JRNL-869265.
- Xue, Xinzhe, Longsheng Feng, Qiu Ren, Cassidy Tran, Samuel Eisenberg, Anica Pinongcos, Logan Valdovinos, Cathleen Hsieh, Tae Wook Heo, Marcus A Worsley, others , Cheng Zhu, and Yat Li. 2024. "Interpenetrated structures for enhancing ion diffusion kinetics in electrochemical energy storage devices." *Nano-Micro Letters* 16, , no. 1 : 255. LLNL-JRNL-862347.
- Sarnecki, Sam. 2025. "Modeling Electrodeposition in 3D Porous Architectures for Solid-State Li-Metal Batteries." *Journal of the Electrochemical Society*. <https://doi.org/10.1149/1945-7111/adfeea>. LLNL-JRNL-2004611.
- Pinongcos, Anica, Xinzhe Xue, Megan C Freyman, Seongkoo Cho, Swetha Chandrasekaran, Qiu Ren, Nathan Delaney, Emma Coester, Marissa Wood, Marcus A Worsley, and others . 2026. "Nitrogen Doping-Enabled Low-Temperature Capacitance Retention in Carbon Materials." *Chemical Communications*. LLNL-JRNL-2011648.
- White, Makena, Minseok Choi, Bintao Hu, Swetha Chandrasekaran, Xinzhe Xue, Marcus Worsley, Yat Li, and Bruce Dunn. 2025. "Recent Advances in Scalable, High-Mass Loaded Electrodes for Grid-Scale Energy Storage." *Advanced Materials*, : 2417128. LLNL-JRNL-871211.
- Lin, Tiras Y, Hanyu Li, Nicholas W Brady, Nicholas R Cross, Victoria M Ehlinger, Thomas Roy, Daniel Tortorelli, Christine Orme, Marcus A Worsley, and Giovanna Bucci. 2024. "Shape matters: understanding the effect of electrode geometry on cell resistance and chemo-mechanical stress." *Journal of the Electrochemical Society* 171, , no. 10 : 100515. LLNL-JRNL-864862.
- Luo, Yunkai, Bintao Hu, Swetha Chandrasekaran, Megan C Freyman, Dun Lin, Yat Li, Marcus Worsley, and Bruce Dunn. 2025. "Stable cycling of high-mass loaded MnO₂ electrodes for sodium-ion batteries." *EES Batteries*. LLNL-JRNL-2010288.
- Rampal, Nikhil, Stephen E Weitzner, Seongkoo Cho, Christine A Orme, Marcus A Worsley, and Liwen F Wan. 2024. "Structural and transport properties of battery electrolytes at sub-zero temperatures." *Energy & Environmental Science* 17, , no. 20 : 7691–7698. LLNL-JRNL-855381.

Ye, Jianchao. 2025. "Superior electrochemical performance and reduced heat generation in 3D printed vs. 2D tape-casted NMC622 electrodes." *Journal of Power Sources*. <https://doi.org/10.1016/j.jpowsour.2024.235861>. LLNL-JRNL-2003168.

Li, Hanyu, Giovanna Bucci, Nicholas W Brady, Nicholas R Cross, Victoria M Ehlinger, Tiras Y Lin, Miguel Salazar de Troya, Daniel Tortorelli, Marcus A Worsley, and Thomas Roy. 2024. "Topology optimization for the full-cell design of porous electrodes in electrochemical energy storage devices." *Structural and Multidisciplinary Optimization* 67, , no. 11 : 188. LLNL-JRNL-862205.

Lin, Tiras. 2025. "Topology Optimization of Curved Electrodes with Suggested Simplified Corrugated Designs." *ACS Electrochemistry*. LLNL-JRNL-2007001.

Luo, Yunkai, Swetha Chandrasekaran, Bintao Hu, Randy Chen, Marcus Worsley, and Bruce Dunn. 2024. "Transforming nanoscale VO₂ (B) into a scalable sodium-ion electrode." *Nano Research* 17, , no. 10 : 8809–8818. LLNL-JRNL-2005949.

Clemens, Auston L, Kyle Jung, Massimiliano Ferrucci, Megan E Ellis, Jonathan T Davis, Swetha Chandrasekaran, Zhen Qi, Christine A Orme, Marcus A Worsley, Rohan Akolkar, and others . 2025. "Understanding the Current Distribution and Mass Transport Properties in 3D-Printed Architected Flow-Through Electrodes." *ACS Applied Engineering Materials* 3, , no. 3 : 600–612. LLNL-JRNL-854706.

Cross, Nicholas R, Hanyu Li, Thomas Roy, Victoria M Ehlinger, Tiras Y Lin, Nicholas W Brady, Swetha Chandrasekaran, Marcus A Worsley, and Giovanna Bucci. 2024. "Viability of Additively Manufactured Electrodes for Lithium-Ion Batteries." *ACS Applied Engineering Materials* 3, , no. 1 : 214–224. LLNL-JRNL- 871091.

Posters

Freyman, Megan. 2023. "Carbon Scaffolds for Energy Storage Applications." (Poster Presentation at DLR Workshop, Livermore, California). LLNL-POST-848091.

Rampal, Nikhil. 2025. "Design principle derived from atomistic simulations for low-temperature functional Li-ion electrolytes." (Poster Presentation at PLS Postdoctoral Symposium, Livermore, California). LLNL-POST-2007675.

Freyman, Megan. 2025. "Effect of Carbon Precursor on electrode Performance." (Poster Presentation at MRS Spring Meeting, Seattle, Washington). LLNL-POST-2004347.

Sun, Wenyu. 2023. "First-principles evaluation of MnO₂ polymorphs as cathode materials in lithium-ion batteries for low temperatures." (Poster Presentation at Battery Workshop, Livermore, California). LLNL-POST-854903.

Song, Youngil. 2023. "Mesoscopic simulations for electrodeposition and electrochemical reaction/diffusion within battery systems for extreme conditions." (Poster Presentation at Battery Workshop, Livermore, California). LLNL-POST-854748.

Brady, Nicholas. 2024. "Modeling Pseudo-Capacitance as Parallel Intercalation and Adsorption Reactions." (Poster Presentation at ECS Spring Meeting, San Francisco, California). LLNL-POST-864425.

Rampal, Nikhil. 2023. "Understanding the 3-phase paradigm using classical molecular dynamics and enhanced sampling simulations." (Poster Presentation at Battery Workshop, Livermore, California). LLNL-POST-854827.

Abstracts

Wood, Marissa. 2025. "3D Electrode Architectures for High Energy Density Batteries." Abstract. *MRS Spring Meeting*, LLNL-ABS-2000805.

Worsley, Marcus Andre, Victor A Beck, Mariana Desiree Reale Batista, Swetha Chandrasekaran, Bryan Moran, Miguel A Salazar de Troya, Adam Carleton, Thomas Roy, Daniel Tortorelli, Michael Stadermann, and others . 2022. "3D Printing of 2D Materials for Optimized Electrochemical Performance." Abstract. *ECS*,no. 12 : 2460–2460. LLNL-ABS-858493.

Brady, Nicholas, Giovanna Bucci, Swetha Chandrasekaran, Sourav Chatterjee, Seongkoo Cho, Auston L Clemens, Nicholas R Cross, Ella Davidi, Victoria Marie Ehlinger, Jeremy Feaster, and others . 2024. "3D Printing of 2D Materials for Optimized Electrochemical Performance." Abstract. *ECS*,no. 12 : 997–997. LLNL-ABS-848511.

Batista, Mariana Desiree Reale, Swetha Chandrasekaran, Bryan Moran, Miguel A Salazar de Troya, Adam Carleton, Thomas Roy, Manhao Zeng, Anica Pinongcos, Dun Lin, Zhen Wang, and others . 2022. "Additive Manufacture of Graphene Electrodes for Supercapacitor Applications." Abstract. *ECS*,no. 1 : 60–60. LLNL-ABS-833297.

Worsley, Marcus Andre. 2025. "Additively Manufactured Carbon Electrodes for Optimized Electrochemical Performance." Abstract. *ECS*,no. 10 : 883–883. LLNL-ABS-871670.

Worsley, Marcus. 2025. "Aerogel Research Highlights from LLNL." Abstract. *NASA Aerogel Lecture Series-Lecture 4*, LLNL-PRES-2010363.

Worsley, Marcus. 2023. "Aerogels, additive manufacturing, and electrochemical energy storage." Abstract. *2nd International Conference on Aerogel Inspired Materials*, LLNL-ABS-848660.

Batista, Mariana Desiree Reale, Swetha Chandrasekaran, Bryan Moran, Miguel A Salazar de Troya, Anica Pinongcos, Zhen Wang, Ryan Hensleigh, Adam Carleton, Manhao Zeng, Thomas Roy, and others . 2024. "Design and Additive Manufacturing of Electrodes for Electrochemical Energy Storage." Abstract. *ECS*,no. 1 : 78–78. LLNL-ABS-XXXXX.

Wan, Liwen, Nikhil Rampal, Stephen Eric Weitzner, Seongkoo Cho, Christine Orme, and Marcus Andre Worsley. 2025. "Design Principle Derived from Atomistic Simulations for Low-Temperature Functional Li-Ion Electrolytes." Abstract. *MRS Spring Meeting*,no. 8 : 856–856. LLNL-ABS-870990.

Bucci, Giovanna, Tiras Y Lin, Nicholas Brady, Nicholas R Cross, Hanyu Li, Victoria Marie Ehlinger, Thomas Roy, Christine Orme, and Marcus Andre Worsley. 2024. "Design Principles for Architected Battery Electrodes." Abstract. *ECS*,no. 2 : 510–510. LLNL-PRES-2000172.

Worsley, Marcus. 2024. "Developing Routes for 3D Printed Aerogel-Inspired Electrodes." Abstract. *22nd International Sol Gel Conference*, LLNL-ABS-858495.

Worsley, Marcus Andre. 2024. "Developing Routes for 3D Printed Carbon Aerogel Electrodes." Abstract. *ECS PRIME Meeting*,no. 11 : 1510–1510. LLNL-PRES-870168.

Worsley, Marcus Andre. 2025. "Electrodeposition into 3D Structures for Electrochemical Energy Storage Applications." Abstract. *ECS*,no. 23 : 1410–1410. LLNL-CFPRES-2006071.

Chandrasekaran, Swetha, Dun Lin, Mariana Desiree Reale Batista, Hanyu Li, Adam Carleton, Xinzhe Xue, Yunkai Luo, Bintao Hu, Bryan Moran, Thomas Roy, and others . 2023. "Graphene-Based Scaffolds for Electrochemical Energy Storage." Abstract. *ECS*,no. 13 : 1299–1299. LLNL-PRES-848393.

Cross, Nicholas R, Tiras Y Lin, Nicholas Brady, Sam Sankar Selvasundarasekar, Hanyu Li, Victoria Marie Ehlinger, Thomas Roy, Marcus Andre Worsley, Rohan Akolkar, Christine Orme, and others . 2025. "Inclusion of a Growing SEI Improves the Ability to Predict Dendrite Formation in Lithium Metal Batteries." Abstract. *ECS*,no. 6 : 725–725. LLNL-CFPRES-2005951.

Li, Hanyu. 2024. "Maximize Energy Storage of Porous Electrodes Using Level-Set Topology Optimization." Abstract. *USNCCM*, LLNL-ABS-871632.

Roy, Thomas, Hanyu Li, Nicholas Brady, Giovanna Bucci, Nicholas R Cross, Victoria Marie Ehlinger, Tiras Y Lin, Miguel A Salazar de Troya, Daniel Tortorelli, and Marcus Andre Worsley. 2024. "Maximizing Energy Density of Full-Cell Storage Devices Using Topology Optimization." Abstract. *ECS*,no. 45 : 2512–2512. LLNL-PRES-864429.

Roy, Thomas, Miguel A Salazar de Troya, Marcus Andre Worsley, and Victor A Beck. 2022. "Maximizing Energy Efficiency of Porous Electrodes Via Topology Optimization." Abstract. *ECS*,no. 46 : 1969–1969. LLNL-ABS-XXXXX.

Cross, Nicholas R, Hanyu Li, Thomas Roy, Victoria Marie Ehlinger, Tiras Y Lin, Nicholas Brady, Swetha Chandrasekaran, Marcus Andre Worsley, and Giovanna Bucci. 2025. "Modeling Additively Manufactured Electrodes to Assess Device-Level Performance in Lithium-Ion Batteries." Abstract. *ECS*,no. 26 : 1469–1469. LLNL-CFPRES-2006080.

Bucci, Giovanna. 2025. "Modeling the effect of electrode geometry, and interface patterning in solid-state batteries." Abstract. *European Solid Mechanics Conference 2025*, LLNL-ABS-2001427.

Ehlinger, Victoria Marie, Nicholas Brady, Seongkoo Cho, Nicholas R Cross, Hanyu Li, Tiras Y Lin, Asya Orhan, Christine Orme, Erika Paola Guzman, Thomas Roy, and others . 2025. "Modeling the Effect of Temperature on the Performance of MnO₂ Electrodes in Lithium-Ion Batteries." Abstract. *ECS*,no. 8 : 813–813. LLNL-CFPRES-2006011.

Ehlinger, Victoria. 2025. "Modeling the Effect of Temperature on the Performance of MnO₂ Electrodes in Lithium-Ion Batteries." Abstract. *ECS*, LLNL-ABS-2001454.

Cross, Nicholas. 2024. "Numerical modeling of 3D printed structures for lithium metal batteries." Abstract. *ECS*, LLNL-ABS-858400.

Roy, Thomas, Nicholas Brady, Giovanna Bucci, Nicholas R Cross, Victoria Marie Ehlinger, Hanyu Li, Tiras Y Lin, and Marcus Andre Worsley. 2025. "Scalable Simulation of the P4D Battery Model for Complex 3D Electrodes." Abstract. *ECS*, no. 26 : 1470–1470. LLNL-CFPRES-2006079.

Bucci, Giovanna. 2024. "Shape matters: Understanding the effect of electrode geometry and microstructure." Abstract. *ECS*, LLNL-ABS-2000792.

Li, Hanyu. 2024. "Shape Optimization for Lithium-Ion Battery with Porous Electrodes." Abstract. *ECS*, LLNL-ABS-857511.

Li, Hanyu. 2024. "Shape Optimization for Lithium-Ion Battery with Porous Electrodes." Abstract. *WCCM*, LLNL-ABS-859070.

Lin, Tiras Y, Thomas Roy, Marcus Andre Worsley, and Giovanna Bucci. 2024. "The Effect of Shape in Porous Electrodes on Cell Resistance and Chemo-Mechanical Stresses." Abstract. *ECS*, no. 2 : 456–456. LLNL-ABS-857536.

Lin, Tiras Y, Hanyu Li, Thomas Roy, Marcus Andre Worsley, and Giovanna Bucci. 2025. "Topology Optimization of Curved Electrodes for Energy Storage." Abstract. *ECS*, no. 26 : 1467–1467. LLNL-ABS-871540.

Orme, Chris. 2022. "Visualizing Growth & Dissolution at Solid-Solution Interfaces." Abstract. *Invited Seminar University of Virginia*, LLNL-ABS-841948.

Presentations

Marcus Worsley, 2023, "3D Printing of 2D Materials for Optimized Electrochemical Performance." (Presented at AIChE Annual Meeting, Orlando, Florida, November 2023).

Marcus Worsley, 2025, "Additive Manufactured Carbon Electrodes for Optimized Electrochemical Performance." (Presented at ECS Meeting, Montreal, Canada, May 2025).

Marcus Worsley, 2025, "Additive Manufacturing of Battery Electrodes." (Presented at Groupement de Recherche, GDR, Redox Flow, CNRS, N/A, September 2025).

Marcus Worsley, 2025, "Additively Manufactured Electrodes for Electrochemical Energy Storage." (Presented at 5th International Conference on Nano Materials for Health, Energy and the Environment (5-ICNM), Pointe aux Piments, Mauritius, September 2025).

Marcus Worsley, 2025, "Advances in Additive Manufacturing of Porous Materials." (Presented at GRC, Andover, New Hampshire, August 2025).

Marcus Worsley, 2025, "Advances in Aerogels and Additive Manufacturing." (Presented at 3rd Aerogel Industry-Academia Forum, Zurich, Switzerland, June 2025).

Marcus Worsley, 2023, "Aerogel, Additive Manufacturing, and Electrochemical Energy Storage'." (Presented at 2nd International Conference on Aerogel Inspired Materials, Donostia-San Sebastian, Spain, September 2023).

Marcus Worsley, 2024, "Aerogels for Energy and Environmental Applications." (Presented at 8th International Summer School on Aerogels, Cologne, Germany, September 2024).

Stephen Weitzner, 2023, "Atomistic modeling of electrochemical Interfaces: Application to energy storage." (Presented at IBM Research Seminar, Almaden, California, October 2023).

Nikhil Rampal, 2024, "Decoding the mechanistic processes that dictate battery performance using enhanced sampling simulations." (Presented at ACS Fall Meeting, Denver, Colorado, August 2024).

Sabrina Wan, 2025, "Design Principle Derived from Atomistic Simulations for Low-T Functional Li-Ion Electrolyte." (Presented at ECS Meeting, Montreal, Canada, May 2025).

Nicholas Cross, 2024, "Design Principles for Architected Battery Electrodes." (Presented at ECS Meeting, San Francisco, California, May 2024).

Nikhil Rampal, 2025, "Design Principles for High-Performance Electrolytes—Overcoming Low-Temperature Challenges in Lithium-Ion Batteries." (Presented at MRS Spring Meeting, Seattle, Washington, April 2025).

Marcus Worsley, 2025, "Developing Methods for Additive Manufacture of Energy Storage Electrodes." (Presented at EMA, Denver, Colorado, February 2025).

Giovanna Bucci, 2023, "Electro-chemo-mechanics and architecture in battery materials from a continuum modeling perspective." (Presented at Battery Workshop, Livermore, California, September 2023).

Giovanna Bucci, 2023, "Electro-chemo-mechanics and architecture in battery materials from a continuum modeling perspective." (Presented at Mitra-Chem Invited Seminar, Mountain View, California, October 2023).

Sabrina Wan, 2023, "Multiscale modeling of electrochemical Interfaces." (Presented at Battery Workshop, Livermore, California, September 2023).

Sabrina Wan, 2023, "Overview of atomistic modeling of battery materials." (Presented at Mitra-Chem Invited Seminar, Mountain View, California, October 2023).

Thomas Roy, 2023, "Topology Optimization for Li-ion Batteries." (Presented at ICIAM, Tokyo, Japan, August 2023).

Thomas Roy, 2024, "Topology optimization for the design of porous electrodes in energy storage devices." (Presented at TOP Webinar, N/A, December 2024).

Tiras Lin, 2025, "Topology optimization of curved electrodes for energy storage." (Presented at ECS Meeting, Montreal, Canada, May 2025).

Nicholas Brady, 2025, "Understanding Charge—Transfer and Storage in Lithium-Ion Pseudo-Capacitor Materials." (Presented at ECS Meeting, Montreal, Canada, May 2025).

Patents

Hensleigh, Ryan. 2024. *Architected three dimensional graphene via additive manufacturing*. Submitted.

Li, Yat. 2025. *Porous Scaffolds and Method for Controlled and Uniform Electrodeposition of Manganese Dioxide Theron*. Submitted.

Records of Invention

Worsley, Marcus. 2025. *Controlled and Uniform Electrodeposition of Manganese Dioxide on 3D Porous Scaffolds*. 2025-288.

23-SI-003: Virtual Inspection of Advanced Manufacturing via Process-Scale Digital Twins

Project Overview

Inspection and certification comprise the most significant bottlenecks in advanced manufacturing for NNSA applications, often requiring far more time and resources than the fabrication of the parts themselves. Traditional methods, such as manual review and X-ray computed tomography, are not only slow and costly, but also struggle to provide a clear connection between manufacturing instructions and the final performance of critical components. This gap limits both the agility and assurance needed to support the modernization and safety of the United States nuclear stockpile.

In response, our Strategic Initiative established a digital twin framework that integrates real-time process monitoring, automated data analysis, and immersive virtual reality (VR) collaboration into a unified inspection pipeline. By leveraging data from sensors, machine instructions, and imaging, we created high-fidelity virtual models of manufactured parts that could be rapidly analyzed and certified. This approach was first demonstrated with Direct Ink Write, and then extended to other manufacturing settings, including conventional (or “subtractive”) manufacturing and to predict the end of life performance of parts per the aging and lifetimes programs. The result is a transformational capability: inspection times have been reduced by a factor of 120,000 without loss of accuracy and while simultaneously improving traceability and confidence in part quality. This framework not only streamlines certification for critical applications, but also positions the national security enterprise to respond more flexibly to emerging challenges, supporting agile manufacturing and digital engineering practices across a broad range of mission-relevant domains.

Mission Impact

The research conducted in this project delivers a transformative impact on LLNL’s core missions by fundamentally accelerating and enhancing the inspection and certification of advanced manufactured components, directly supporting the safety, security, and effectiveness of the U.S. nuclear weapons stockpile. By developing a robust digital twin framework that integrates process- and part-scale modeling, data-driven analytics, and immersive virtual reality, this work enables rapid, traceable, and data-rich part qualification—addressing one of the most significant bottlenecks in the NNSA’s manufacturing enterprise. The new capabilities pioneered here not only reduce production cycle times and resource demands, but also establish a foundation for agile, adaptive manufacturing and digital engineering practices across the Laboratory. The project’s outcomes have already seeded new research directions in machine learning-driven process monitoring, advanced computed tomography (CT) inspection, and collaborative VR-based virtual reality analysis, attracting new staff and fostering multidisciplinary collaborations. Beyond LLNL, these advances are highly relevant to DOE/NNSA missions by providing scalable tools for stockpile modernization, nonproliferation, and the agile response to emerging national security challenges. The framework’s extensibility to other advanced and conventional manufacturing modalities further positions LLNL and its partners to lead in digital engineering and mission assurance, while the demonstrated VR tools and data pipelines offer potential benefit to other federal agencies charged with critical infrastructure, emergency response, and technology innovation. Collectively, this project exemplifies LLNL’s commitment to

developing science and technology tools and capabilities to meet current and future national security needs.

Publications, Presentations, and Patents

Hernandez, Kristen, Erika Barcelos, Jayvic Jimenez, Arafath Nihar, Pawan Tripathi, Brian Giera, Roger French, and Laura Bruckman. 2025. "A data integration framework of additive manufacturing based on FAIR principles." *MRS Advances* 9, , (May): 844–851. LLNL-JRNL-857803.

Ojal, Nishant, Pigeon Caviness, Alex Blum, Brian Au, Adam Jaycox, and Brian Giera. 2024. "Optimizing exposure times of structured light metrology systems using a digital twin." *Measurement* 224, , (January): 113816. LLNL-JRNL-845220.

Aung, Hein, Jayvic Jimenez, Brian Au, Pigeon Caviness, Robert Cerda, Quynh Tran, Pawan Tripathi, Brian Giera, Roger French, and Laura Bruckman. 2024. "Towards a study protocol: A data-driven workflow to identify error sources in direct ink write mechatronics." *MRS Advances* 9, , (May): 837–843. LLNL-JRNL-85917.

Chheang, Vuthea, Brian Weston, Robert Cerda, Brian Au, Brian Giera, and P-T Bremmer. 2024. "A Virtual Environment for Collaborative Inspection in Additive Manufacturing." In the Proceedings of CHI EA '24: Extended Abstracts of the CHI Conference on Human Factors in Computing Systems, CHI EA '24, May. <https://doi.org/10.1145/3613905.3650730>. LLNL-PROC-859114.

Rodrigues, Francielly, Alexander Giovannelli, Leonardo Pavanatto, Haichao Miao, Jauvane Oliveira, and Bowman Bowman. 2023. "AMP-IT and WISDOM: Improving 3D Manipulation for High-Precision Tasks in Virtual Reality." In the Proceedings of 2023 IEEE International Symposium on Mixed and Augmented Reality, ISMAR, December. <https://doi.org/10.1109/ismar59233.2023.00045>. LLNL-CONF-850723.

Ai, Kuangshi, Haichao Miao, Zhimin Li, Chaoli Wang, and Shusen Li. 2025. "An Evaluation-Centric Paradigm for Scientific Visualization Agents." In the Proceedings of IEEE VIS Conference 2025, : 1st Workshop on GenAI, Agent. <https://doi.org/10.48550/arxiv.2509.15160>. LLNL-CONF-2010304.

Liu, Shusen, Haichao Mia, Zhimin Li, Matthew Olson, Valerio Pascucci, and P-T Bremmer. 2024. "AVA: towards autonomous visualization agents through visual perception-driven decision-making." In the Proceedings of Computer Graphics Forum, Eurographics Conference on Visualization, June. <https://doi.org/10.1111/cgf.15093>. LLNL-CONF-857838.

Kutak, David, Danielle Langlois, Roman Rozic, Jan Byska, Haichao Miao, Simone Kriglstein, and Barbara Kozlikova. 2024. "Design and evaluation of alphabetic and numeric input methods for virtual reality." In the Proceedings of Computers & Graphics, Technical Section, August. <https://doi.org/10.1016/j.cag.2024.103955>. LLNL-CONF-850222.

Pavanatto, Leonardo, Alexander Giovannelli, Brian Giera, P-T Bremmer, Haichao Miao, and Doug Bowman. 2025. "Exploring Multiscale Navigation of Homogeneous and Dense Objects with Progressive Refinement in Virtual Reality." In the Proceedings of 2025 IEEE Conference Virtual

Reality and 3D User Interfaces, IEEE Conference Virtual Reality and 3D User Interfaces, March. LLNL-CONF-863666.

Giovannelli, Alexander, Leonardo Pavanatto, Shakiba Davari, Haichao Miao, Vuthea Chheang, and Brian Giera. 2025. "Investigating the Influence of Playback Interactivity during Guided Tours for Asynchronous Collaboration in Virtual Reality." In the Proceedings of 2025 IEEE Conference Virtual Reality and 3D User Interfaces (VR), Saint Malo, France. LLNL-CONF-869200.

Miao, Haichao, Saurabh Narain, Vuthea Chheang, Garrett Hooten, Raiyan Seede, Pavol Klacansky, Kaila Morgen Bertsch, Gabe Guss, Brian Giera, and Peer-Timo Bremer. 2025. "LatticeAnalytics: Strut-Level Visualization and Inspection of Additively Manufactured Lattice Structures." *IEEE Transactions on Visualization and Computer Graphics* 31, , no. 10 : 9266-9283.<https://doi.org/10.1109/tvcg.2025.3593230>. LLNL-JRNL-871130.

Ferrucci, Massimiliano, Anne-Franoise Obaton, Robert Cerda, Brian Au, Nicholas Rodriguez, Ziad Ammar, Gabriel Balensiefer, Chuck Divin, Jeremy Lenhardt, and Brian Giera. 2025. "Measuring thermal curing induced shrinkage of material extrusion based additive manufacturing silicone elastomer lattices by X-ray computed tomography." *Tomography of Materials and Structures* 8, , (June): 100064.<https://doi.org/10.1016/j.tmater.2025.100064>. LLNL-JRNL-2006488.

Abstracts

Chheang, Vuthea, Brian Weston, Robert Cerda, Brian Au, Brian Giera, Peer-Timo Bremer, and Haichao Miao. 2024. "A Virtual Environment for Collaborative Inspection in Additive Manufacturing." Abstract. *CHI EA '24: Extended Abstracts of the CHI Conference on Human Factors in Computing Systems*, no. 26 (May): 1-7.<https://dl.acm.org/doi/full/10.1145/3613905.3650730>. LLNL-PROC-859114.

Code

Watts, Seth, and Sam Mish. 2023. *Mesh from part data*.

23-SI-005: Protective Host-Targeted Engineered Gene Therapeutics

Project Overview

Prepositioned countermeasures are urgently needed to combat viral pandemics. Conventional post-emergence virus-targeted therapies require considerable lead time, increasing the number of patients who may experience serious illness and death. We assembled a multidisciplinary team to fundamentally change the pandemic preparedness paradigm by enabling pre-emptive development of a new class of broadly protective, host-targeted therapeutics. To do so, we developed an innovative strategy to identify the human host factors that viruses rely on for replication using an integrated artificial intelligence/machine learning (AI/ML) target prediction pipeline. These host factors represent attractive targets for therapy as they are genetically more stable than viral targets and may be shared among related viruses. However, they have not been well-explored due to (a) lack of precise knowledge of complex, networked host-virus interactions, and (b) lack of availability of therapeutic modalities for safe host gene modulation. Specifically, we developed active learning algorithms to integrate side information in the form of biological knowledge graphs with data from large-scale genetic screens in a way that systematically identifies optimal gene target combinations in minimal experimental time. In parallel, we developed enveloped delivery vehicles (EDVs), a novel platform based on pseudotyped lentiviruses, for targeted delivery of epigenome-oriented therapeutics to the human airway. Together, these discoveries advanced the state-of-the-art in versatile platform technologies for countering emerging viral threats.

Mission Impact

While multiplexed targeting of human genes for antiviral prophylaxis or therapy remains a distant, aspirational goal, aspects of PROTECT have provided an outline for a rapid and versatile antiviral platform centered around components of the host genome. Delivery vehicles developed in the course of this project have also advanced the feasibility of specifically targeting airway tissue, supporting diverse intervention modalities. Ultimately, steps toward the creation of a platform capable of learning and manipulating host-pathogen interactions at genome scale, with quantifiable predictive accuracy, support the development of broadly protective countermeasures in line with LLNL's Bio Resilience Mission Focus Area (MFA) and national infectious disease preparedness goals.

Publications, Presentations, Patents

Soper, Braden, Michal Lisicki, Mary Silva, Jose Cadena, Haonan Zhu, Shivshankar Sundaram, Priyadip Ray, and Jeff Drocco. 2025. "Knowledge graph-aided Bayesian active learning for top- K genetic interaction discovery." *Nature Scientific Reports* 15: Article 31196. <https://doi.org/10.1038/s41598-025-13972-7>

Zhu, Haonan, Mary Silva, Jose Cadena, Braden Soper, Michal Lisicki, Braian Peetoom, Sergio Baranzini, Shivshankar Sundaram, Priyadip Ray, and Jeff Drocco. 2025. "Deep Active Learning based Experimental Design to Uncover Synergistic Genetic Interactions for Host Targeted Therapeutics." *Bioinformatics Advances* Article vbaf228. <https://doi.org/10.1093/bioadv/vbaf228>

Hou, Jiakai, et al. 2024. "Integrated multi-omics analyses identify anti-viral host factors and pathways controlling SARS-CoV-2 infection." *Nature Communications* 15: Article 109.
<https://doi.org/10.1038/s41467-023-44175-1>

23-SI-006: Predictive Atomistic Materials Simulations with Uncertainty Quantification

Project Overview

This project aimed to develop an automated software framework to enable quantum-accurate atomistic materials simulations at billion-atom scale by fitting accurate interatomic potentials (IAPs) with quantified uncertainty. Such a capability allows predictive, quantitative simulations of complex physical and chemical responses of materials over a wide variety of conditions relevant to DOE and to broader science and technology missions. The main outcome of this project was the development and open-source release of the Orchestrator software, which is a Python framework that streamlines the process of training optimal IAPs for accurate materials simulations of interest. The software provides an enabling capability for NNSA and the broader atomistic simulation community, effectively increasing the accessible length and time scales of quantum-accurate simulations by orders of magnitude. To achieve this capability, several enabling techniques were invented during the project and are included within the Orchestrator suite. Key developments included: the *Quick Uncertainty and Entropy via Structural Similarity (QUESTS)* methodology to analyze and remove redundancy in training datasets, measure dataset completeness, and detect out-of-domain anomalies during simulations; the *Loss Trajectory Analysis for Uncertainty in atomistic Force Fields (LTAU-FF)* methodology to efficiently estimate training uncertainty; the *Multi-kernel Edge Attention Graph Autoencoder (MEAGraph)* methodology to cluster together similar atomic environments; the *Information Matching for Active Learning (IMAL)* methodology that uses Fisher information theory to optimize IAP training to bound the uncertainty of a target property prediction. In addition, a co-optimization procedure was developed to create bespoke IAPs that are specially tuned for highly-accurate prediction of “indicator properties” so that large-scale simulations accurately predict a complex property of interest. Finally, a machine learning methodology was developed that allows acceleration of molecular dynamics simulations by a factor of 10 to 100.

The tools developed in this project were applied to study various material systems under extreme conditions. For example, we explored the viscosity of liquid carbon at high pressures, temperature, and strain rates relevant to planetary science, finding an appreciable increase in the viscosity when supercooled below the diamond melting line; we also studied the formation and phase evolution of nanocarbon during detonation conditions. We explored highly energetic chemical pathways in compressed mixtures of carbon, nitrogen, and oxygen to understand nucleation in contrails. We also computed accurate, uncertainty-quantified high-pressure melt lines of iron, nickel, and iron-nickel mixtures, relevant for understanding the nature of the Earth’s core. A database built-in to the Orchestrator software stores and tracks all training data and materials models created, facilitating later access to the data as well as eliminating duplication of computational effort by enabling reuse of prior simulations.

Mission Impact

The capability developed by this project expands the range of applicability of quantitatively accurate atomistic simulations for materials critically relevant to the NNSA stockpile stewardship and broader missions. With their uncertainties quantified, these atomistic simulations can reliably augment lengthy and costly experiments, reducing the number of experiments required. Combined

with the world-leading high-performance computing capability at LLNL, these tools position LLNL to meet future national security challenges, both for NNSA's mission as well as DOE's broader energy security mission. The products of this project are currently being leveraged for a newly-awarded Artificial Intelligence for Nuclear Security (AI4NS) project at LLNL sponsored by the NNSA Advanced Simulation and Computing Program (ASC).

Publications

Lindsey, Rebecca, Sorin Bastea, Sebastien Hamel, Yanjun Lyu, Nir Goldman, and Vincenzo Lordi. 2025. "ChIMES Carbon 2.0: A Transferable Machine-Learned Interatomic Model Harnessing Multifidelity Training Data." *npj Computational Materials* 11, (February): 26. <https://doi.org/10.1038/s41524-024-01497-y>. LLNL-JRNL-861515.

Jaspersen, Benjamin, Iliia Nikiforov, Amit Samanta, Fei Zhou, Ellad Tadmor, Vincenzo Lordi, and Vasily Bulatov. 2025. "Cross-scale covariance for material property prediction." *npj Computational Materials* 11, (January): 1. <https://doi.org/10.1038/s41524-024-01453-w>. LLNL-JRNL-860766.

Zhao, Liming, Sebastien Hamel, Vincenzo Lordi, and Amit Samanta. 2024. "High Pressure Melt Line of Nickel Using a Generalized Embedded Atomic Method Potential." *Applied Physics Letters* 124: 234102. LLNL-JRNL-859706.

Sun, Hong, Sebastien Hamel, Tim Hsu, Babak Sadigh, Vincenzo Lordi, and Fei Zhou. 2024. "Ice phase classification made easy with score-based denoising." *Journal of Chemical Information and Modeling* 64: 6369. <https://doi.org/10.1021/acs.jcim.4c00822>. LLNL-JRNL-862778.

Vita, Joshua, Amit Samanta, Fei Zhou, and Vincenzo Lordi. 2025. "LTAU-FF: Loss Trajectory Analysis for Uncertainty in atomistic Force Fields." *Machine Learning: Science & Technology* 6, (February): 015048. <https://doi.org/10.1088/2632-2153/adb4b9>. LLNL-JRNL-860048.

Willman, Jonathan, Joseph Gonzalez, Kien Nguyen-Cong, Sebastien Hamel, Vincenzo Lordi, and Ivan Oleynik. 2024. "Machine Learning Interatomic Potential for Simulations of Carbon at Extreme Conditions." *Journal of Chemical Physics* 161: 084709. LLNL-JRNL-860046.

Zhao, Liming, Vincenzo Lordi, and Amit Samanta. 2024. "Melting Point of Iron at High Pressure: An assessment of uncertainties and effect of electronic temperature." *Applied Physics Letters* 124: 144105. LLNL-JRNL-855137.

Schwalbe-Koda, Daniel, Sebastien Hamel, Babak Sadigh, Fei Zhou, and Vincenzo Lordi. 2025. "Model-free estimation of completeness, uncertainties, and outliers in atomistic machine learning using information theory." *Nature Communications* 16, (April): 4014. <https://doi.org/10.1038/s41467-025-59232-0>. LLNL-JRNL-862887.

Kwon, Hyuna, Tim Hsu, Wenyu Sun, Wonseok Jeong, Fikret Aydin, James Chapman, Xiao Chen, Vincenzo Lordi, Matthew Carbone, Deyu Lu, Fei Zhou, and Tuan Pham. 2024. "Spectroscopy-Guided Discovery of Three-Dimensional Structures of Disordered Materials with Diffusion Models." *Machine Learning: Science and Technology* 5:045037 (November). <https://doi.org/10.1088/2632-2153/ad8c10>. LLNL-JRNL-858133.

Laubach, Benjamin, Vincenzo Lordi, and Rebecca Lindsey. 2026. "Cluster-Graph Fingerprinting: A Framework for Quantitative Analysis of Machine-Learned Interatomic Model Training and Simulation Data." *Journal of Chemical Information and Modeling* 66:182. <https://doi.org/10.1021/acs.jcim.5c02179>. LLNL-JRNL2005542.

Wang, Kaiyang, Vincenzo Lordi, Stephan Friedrich, and Amit Samanta. 2026. "Development of an interatomic potential for the Ta-Li system." *Computational Materials Science* 263, (February): 114393. <https://doi.org/10.1016/j.commatsci.2025.114393>. LLNL-JRNL-2005266.

Jaspersen, Benjamin, Ilia Nikiforov, Amit Samanta, Brandon Runnels, Harley Johnson, and Ellad Tadmor. 2025. "Fundamental microscopic properties as predictors of large-scale quantities of interest: Validation through grain boundary energy trends." *Acta Materialia* 286, (March): 120722. <https://doi.org/10.1016/j.actamat.2025.120722>. LLNL-JRNL-867022.

Copley, Jonathan, and Sebastien Hamel. 2025. "Overcoming time and complexity limitations in molecular dynamics investigations of equilibrium melting." *Modeling and Simulation in Materials Science & Engineering* 33:045011. <https://doi.org/10.1088/1361-651x/add282>. LLNL-JRNL-862625.

Hamel, Sebastien, and Alfredo Correa. 2025. "The transformative capability of quantum-accurate machine learning interatomic potentials." *KIM Review* 3:01 (May): 1. <https://doi.org/10.25950/ce4db4e8>. LLNL-JRNL-2005837.

Kurniawan, Yonatan, Ben Francis, Tracianne Neilsen, Mark K. Transtrum, Mingjian Wen, Ilia Nikiforov, Ellad Tadmor, Vasily Bulatov, and Vincenzo Lordi. "An information-matching approach to optimal experimental design and active learning." *Applied Physics Letters* in press (2026). <https://doi.org/10.48550/arXiv.2411.02740>. LLNL-JRNL-871052.

Sun, Hong, Joshua Vita, Amit Samanta, and Vincenzo Lordi. "Unsupervised Atomic Data Mining via Multi-Kernel Graph Autoencoders for Machine Learning Potentials." *Machine Learning: Science & Technology* in press (2026). <https://doi.org/10.48550/arXiv.2509.12358>. LLNL-JRNL-863300

Posters

Kurniawan, Yonatan, Mark Transtrum, and Vincenzo Lordi. 2023. "Indicator configurations: An information-matching method of data reduction for training interatomic potential." (Poster Presentation at SES Annual meeting, Minneapolis, MN, October). LLNL-POST-849700.

Sundberg, Brayden, Sebastien Hamel, Vincenzo Lordi, and Rebecca Lindsey. 2025. "Toward Simulation of Silicon-Nanoparticle Shock-Synthesis Using Machine-Learned Interatomic Potentials." (Poster Presentation at APS SCCM Meeting 2025: 24th International Conference on the Science of Compression in Condensed Matter, Washington, D.C., June). LLNL-POST-2007065.

Abstracts

Kurniawan, Yonatan, Vasily Bulatov, Benjamin Jasperson, Ilia Nikiforov, Ellad Tadmor, Mark Transtrum, and Vincenzo Lordi. 2023. "Indicator configurations: An information-matching method for efficient data selection in interatomic potential training." Abstract. *APS Four Corners Meeting*, (October). LLNL-ABS-854797.

Samanta, Amit, Tianjiao Li, Weishi Wang, Mark Transtrum, and Vincenzo Lordi. 2024. "Analysis of systematic uncertainties in interatomic potentials." Abstract. *SIAM Conference on Uncertainty Quantification: mini-symposium on Uncertainty Quantification for Active Learning in Atomistic Modeling*, (February). LLNL-ABS-855432.

Presentations

Vasily Bulatov, Ben Jasperson, Ellad Tadmor, Ilia Nikiforov, Amit Samanta, Fei Zhou, Vincenzo Lordi, 2024, "Cross-scale covariance for material property predictions." (Presented at The 11th International Conference on Multiscale Materials Modeling (MMM11), Prague, Czech Republic, September 2024).

Vincenzo Lordi, Daniel Schwalbe-Koda, Fei Zhou, 2023, "Identifying and Quantifying Uncertainty in Fitted Interatomic Potentials for Molecular Dynamics." (Presented at Advancing Molecules and Materials via Data Science, Minneapolis, MN, September 2023).

Yonatan Kurniawan, Vasily Bulatov, Benjamin Jasperson, Ilia Nikiforov, Ellad Tadmor, Mark Transtrum, Vincenzo Lordi, 2023, "Indicator configurations: An information-matching method for efficient data selection in interatomic potential training." (Presented at APS Four Corners Meeting, Logan, UT, October 2023).

Yonatan Kurniawan, Mark Transtrum, Vincenzo Lordi, 2024, "Indicator Configurations: An Information-Matching Method of Data Reduction for Training Interatomic Potential." (Presented at SIAM Conference on Mathematical Aspects of Materials Science (MS24), Pittsburgh, PA, May 2024).

Rebecca Lindsey, 2024, "Leveraging Machine-Learned Interatomic Models for Quantum Accurate Carbon Melt Line Prediction." (Presented at APS March Meeting, Minneapolis, MN, March 2024).

Nicholas Wimer, 2024, "Comparison of Uncertainty Quantification Methods for Scientific Machine Learning." (Presented at AIRES 5, Richland, WA, May 2024).

Tomorr Haxhimali, 2023, "Correlation functions for viscosity and diffusion in dense plasmas." (Presented at Charged-Particle in High Energy Density Plasmas Workshop, Livermore, CA, July 2023).

Benjamin Jasperson, Ilia Nikiforov, Amit Samanta, Fei Zhou, Brandon Runnels, Harley Johnson, Vincenzo Lordi, Vasily Bulatov, Ellad Tadmor, 2025, "Cross-scale covariance for material property prediction." (Presented at Engineering Mechanics Institute Conference, Anaheim, CA, May 2025).

Ellad Tadmor, Benjamin Jasperson, Ilia Nikiforov, Amit Samanta, Fei Zhou, Brandon Runnels, Harley Johnson, Vincenzo Lordi, Vasily Bulatov, 2025, "Cross-scale covariance for material property prediction." (Presented at APS Global Physics Summit 2025, Anaheim, CA, March 2025).

Nicholas Wimer, Juliane Mueller, Sebastien Hamel, Vincenzo Lordi, 2025, "Examining Uncertainty Quantification Techniques for Machine Learned Interatomic Potentials." (Presented at APS Global Physics Summit, Anaheim, CA, March 2025).

Fei Zhou, 2025, "Grand Canonical Generative Diffusion Model for Crystalline Phases and Grain Boundaries." (Presented at TMS Annual Meeting & Exhibition, Las Vegas, NV, March 2025).

Yonatan Kurniawan, Mark Transtrum, Cody Petrie, Dylan Bailey, Vincenzo Lordi, 2023, "Indicator configurations: An information-matching method for efficient data selection in interatomic potential training." (Presented at American Physical Society March Meeting, Las Vegas, NV, March 2023).

Yonatan Kurniawan, Mark Transtrum, Vincenzo Lordi, 2024, "Indicator configurations: An information-matching method of data reduction for training interatomic potential." (Presented at SIAM Conference on Uncertainty Quantification: mini-symposium on Uncertainty Quantification for Active Learning in Atomistic Modeling, Trieste, Italy, February 2024).

Joshua Vita, 2025, "Loss Trajectory Analysis for Uncertainty in Atomistic Force Fields." (Presented at Materials Research Society Fall Meeting, Boston, MA, December 2025).

Brayden Sundberg, Sebastien Hamel, Vincenzo Lordi, Rebecca Lindsey, 2025, "Machine-Learning Interatomic Potentials for Predictive Simulations of Laser-Driven Silicon Nanoparticle Synthesis." (Presented at APS SCCM Meeting 2025: 24th International Conference on the Science of Compression in Condensed Matter, Washinton, D.C., June 2025).

Daniel Schwalbe-Koda, 2025, "Model-free Quantification of Completeness, Uncertainties, and Outliers in Atomistic Machine Learning Using Information Theory." (Presented at SIAM Conference on Computational Science and Engineering, Fort Worth, TX, March 2025).

Daniel Schwalbe-Koda, 2025, "Model-free quantification of completeness, uncertainties, and outliers in atomistic machine learning using information theory." (Presented at APS Global Physics Summit, Anaheim, CA, March 2025).

Kyle Bushick, Fikret Aydin, Josh Vita, Nathan Keilbart, Logan Williams, Eric Fuemmeler, Amit Gupta, Claire Water, Ilia Nikiforov, Yonatan Kurniawan, Ellad Tadmor, Tomas Ooppelstrup, Vincenzo Lordi, 2025, "Orchestrating Interatomic Potential Training and Analysis." (Presented at APS Global Physics Summit 2025, Anaheim, CA, March 2025).

Kyle Bushick, Fikret Aydin, Josh Vita, Nathan Keilbart, Logan Williams, Eric Fuemeller, Amit Gupta, Claire Waters, Ilia Nikiforov, Yonatan Kurniawan, Ellad Tadmor, Tomas Ooppelstrup, Vincenzo Lordi, 2025, "Orchestrating Interatomic Potential Training and Analysis." (Presented at MRS Spring Meeting & Exhibit, Seattle, WA, April 2025).

Kyle Bushick, Fikret Aydin, Marcos Calegari Andrade, Eric Fuemmeler, Amit Gupta, Claire Waters, Ellad Tadmor, Tomas Ooppelstrup, Vincenzo Lordi, 2024, "Orchestrating Interatomic Potential

Training and Analysis." (Presented at The Role of Theories, Simulation, and Machine Learning in Materials Discovery (Gordon Research Conference and Seminar), Newry, ME, July 2024).

Joshua Vita, 2025, "Practical Uncertainty Quantification for Deep Learning Atomistic Force Fields." (Presented at Machine Learning in Chemical and Materials Sciences 2025 (MLCM-25), Santa Fe, NM, May 2025).

Fei Zhou, 2023, "Probabilistic approach to materials modeling." (Presented at TMS Annual Meeting, San Diego, CA, March 2023).

Ellad Tadmor, 2025, "Revolutionizing Molecular Simulation of Materials: The Rise of Data." (Presented at CEMS Seminar, Minneapolis, MN, April 2025).

Yanjun Lyu, Sorin Bastea, Sebastien Hamel, Vincenzo Lordi, Rebecca Lindsey, 2025, "Toward a detailed description of shockwave-driven carbon condensation: Insights from machine-learning-accelerated simulations." (Presented at 24th International Conference on the Science of Compression in Condensed Matter (SCCM 2025), Washington, D.C., June 2025).

Rebecca Lindsey, 2025, "Toward a detailed description of shockwave-driven carbon condensation: Insights from machine-learning-accelerated simulations." (Presented at 24th International Conference on the Science of Compression in Condensed Matter (SCCM 2025), Washington, D.C., June 2025).

Code

Vita, Joshua. 2024. *LTAU-FF: Loss Trajectory Analysis for Uncertainty in atomistic Force Fields*. <https://github.com/LLNL/ltau-ff/>.

Sun, Hong. 2024. *MEAGraph: Multi-kernel Edge Attention Graph Autoencoder*. <https://lc.llnl.gov/gitlab/sun36/meagraph/>.

Schwalbe-Koda, Daniel. 2024. *QUESTS: Quick Uncertainty and Entropy via Structural Similarity*. <https://github.com/dskoda/quests>.

Bushick, Kyle, Joshua Vita, Logan Williams, Claire Waters, Fikret Aydin, Eric Fuemmeler, Nathan Keilbart, Ilia Nikiforov, Amit Gupta, ShinYoung Kang, Yonatan Kurniawan, Jared Stimac, Huy Pham, Nicholas Wimer, Marcos Calegari Andrade, Tomas Opplestrup, Ellad Tadmor, and Vincenzo Lordi. 2025. *Orchestrator*. <https://github.com/LLNL/orchestrator>.