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Lawrence Livermore National Laboratory

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FY24 LDRD Annual Report PDF

A Mosley

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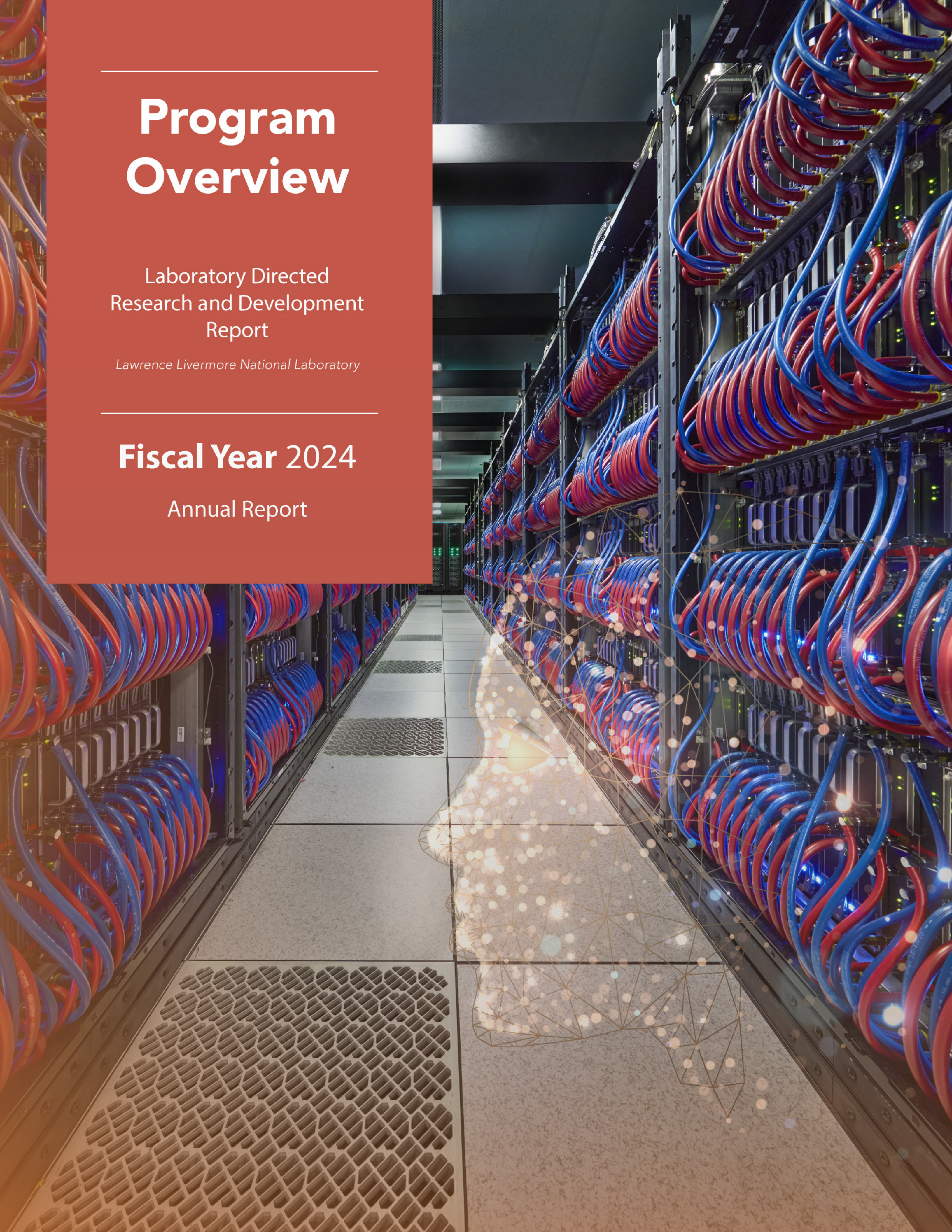
Program Overview

Laboratory Directed Research and Development Report

Lawrence Livermore National Laboratory

Fiscal Year 2024

Annual Report



Annual Program Overview

Director's Statement

Kimberly S. Budil
LLNL Director

The Laboratory Directed Research and Development (LDRD) Program at Lawrence Livermore National Laboratory (LLNL) is the Lab's most significant resource for supporting internally directed research and development. It provides investments in cutting-edge science, technology, and engineering. This program expands the frontiers of knowledge, creates capabilities required by our evolving mission needs, and attracts and retains the world's most talented scientists and engineers. In this annual report, we describe the LDRD investment portfolio, provide information to demonstrate the program's value and impact to LLNL's science, technology and engineering capabilities, and showcase LDRD accomplishments across the Lab's mission space.

The Lab's LDRD Program advances research and development across all LLNL mission and core competencies from biology and high-performance computing to data science and nuclear deterrence. As we continue this broad advancement across all of LLNL's mission space, we remain committed to our focus on areas that are especially critical to our evolving national security and nuclear deterrence mission. The continued success in achieving fusion ignition at the National Ignition Facility advances critical insights into physics at extreme conditions that are essential to key LLNL nuclear deterrence missions. Looking forward, we are driving innovations that will help attain the next frontier of high yield facilities needed for mission deliverables, and that concurrently advance the technical capabilities required for an inertial fusion energy power plant. Advanced Materials and Manufacturing remains at the heart of solutions to our most critical mission needs. We are shortening the time needed to bring a new material from discovery, to design, then to manufacture at scale, in order to provide nimble and agile delivery of mission-required components that can be rapidly certified. Equally and vitally important, advances in artificial intelligence (AI) are progressing at an astounding pace; we see AI as a powerful catalyst to accelerate innovation across all LLNL missions and capabilities. Our work involves partnerships across the science and industrial complex, advances fundamental AI algorithms, and uses AI to deliver new science, technology and engineering.

Spanning LLNL's missions, LDRD investments bring together teams and collaborators to push the frontiers of science, technology, and engineering. This ensures the technical vitality of the Laboratory that is essential to global and national security. For example, one LDRD project is developing new tools, methodologies and a scientific framework to streamline the development-to-production cycle and diversify manufacturing options for high explosives. Another LDRD project is developing an artificial intelligence-enhanced molecular-design assistant trained to understand molecular chemistry to accelerate the discovery of methods to synthesize energetic molecules with optimized characteristics. The LDRD Program cultivates the creativity of the Lab's most important resource—our workforce. LDRD-sponsored research reaches out to tomorrow's innovators, by mentoring students, challenging our postdoctoral researchers, and developing the leadership capabilities of early career staff.

As you browse this report, you will learn about cover-page publications, patents, and science awards that resulted from LDRD investments. Looking ahead, we will continue to innovate science, technology, and engineering solutions to help LLNL remain at the forefront of research and development, positioning us to solve the most complex global and national security challenges.

ldrd-annual.llnl.gov

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Lawrence Livermore National Laboratory

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LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

Program Description

The LDRD program's targeted investments allow LLNL to develop cutting-edge capabilities and foster innovation in key programmatic areas.

Technical Vitality

Mission Agility

Workforce Development

Mission Alignment

Congress established the Laboratory Directed Research and Development (LDRD) Program in 1991 to foster cutting-edge scientific and technical vitality at U.S. Department of Energy (DOE) laboratories. The LDRD Program at each laboratory is a unique resource, providing funding for critical research aimed at addressing today's needs and tomorrow's challenges. LLNL's program addresses DOE objectives, while also aligning with National Nuclear Security Administration (NNSA) mission objectives and the Laboratory's own strategic priorities.

As articulated in DOE Order 413.2C, the LDRD program serves to:

- Maintain the scientific and technical vitality of the laboratories.
- Enhance the laboratories' ability to address current and future DOE/NNSA missions.
- Foster creativity and stimulate exploration of forefront areas of science and technology.
- Serve as a proving ground for new concepts in research and development.
- Support high-risk, potentially high-value research and development.

Alignment with NNSA Mission Objectives

A strategic framework—created jointly by NNSA, LLNL, and the other NNSA laboratories—articulates the focus of LDRD programs at NNSA laboratories. LDRD investments support the following NNSA objectives:

- Technical Vitality. Develop innovative capabilities that are required to respond to emerging national security challenges.
- Mission Agility. Enable agile responses to national security challenges by investing in research and development at the forefront of mission-critical science and technology.
- Workforce Development. Recruit, develop, and retain the best and brightest staff, who can help us creatively address tomorrow's dynamic mission needs.

Alignment with Laboratory Missions

In addition to aligning our LDRD investments with DOE and NNSA objectives, we ensure that our LDRD program supports mission priorities articulated in LLNL's annual strategic investment plan. Institutional goals are established and updated through a planning process where multidisciplinary teams identify:

- Mission-related challenges or areas of interest for high-priority research.
- The core competencies that support this high-priority research.
- The scientific and technological needs to address those challenges and enhance related competencies.
- Key topics in fundamental research.

Program Oversight

Day-to-day oversight of our program is provided by LDRD Program Director Doug Rotman. Overall program oversight extends beyond the LDRD program office to include the LLNL Director and the LLNL Deputy Director for Science and Technology, along with the Laboratory's scientific and programmatic leaders. This Laboratory team works closely with NNSA's Livermore field office, NNSA's LDRD program leaders, and LDRD program leaders at the Department of Energy.

At the programmatic level, LDRD portfolio management at Livermore is structured to assure alignment with DOE, NNSA, and Laboratory missions. Designated LDRD points of contact for each of the Laboratory's strategic investment areas provide input regarding LDRD investment priorities to Livermore's senior leadership team. These points of contact also advise applicants for LDRD funding regarding the alignment between proposed research and evolving mission needs at our Laboratory.

In addition, programmatic leaders and science and technology leaders participate in a rigorous peer-review process of all proposals for LDRD funding. They evaluate the strategic relevance of each proposal, as well as its technical content. NNSA reviews and concurs on funding decisions. Funded projects are periodically reviewed by senior staff to ensure technical success and continued alignment with mission objectives

PERFORMANCE ASSESSMENT

The LDRD program achieves continuous improvement through internal and external reviews of the program, along with oversight of each LDRD research project.

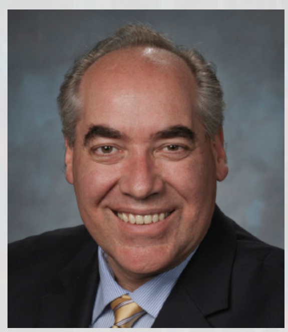
Representatives from LDRD programs at each NNSA laboratory regularly participate in working groups to share best practices and discuss strategies for tracking the long-term impact of LDRD investments.

To assess continued LDRD performance, the LDRD program tracks a suite of short-term and long-term metrics. These performance metrics can be found in the Program Value section of this report and address scientific publications, intellectual property, collaborations, and support for early career staff. Also included are NNSA guided metrics for assessing the long-term impact of LDRD on laboratory staff and capabilities. Our report also includes performance indicators specified by DOE's director of LDRD programs, in accordance with DOE Order 413.2C.

PATRICIA FALCONE

LLNL Deputy Director for Science & Technology

LLNL's Investment Strategy for Science and Technology is updated annually to reflect evolving mission needs, under the guidance of LLNL's deputy director for science and technology. It sets the strategic context for LLNL's annual call for LDRD proposals, and it serves as a resource for investigators as they articulate the ways their proposed research aligns with at least one of these investment priorities.



DOUG ROTMAN

LDRD Program Director

"The LDRD program is an investment in our nation's future, with a mission impact that is often realized many years after an LDRD-sponsored project concludes. I'm extremely proud of everyone at LLNL—from postdocs who serve on LDRD-funded research teams, to senior scientists who help shape our investment strategy—so that together, we can ensure that the LDRD program continues to serve as a valuable national asset."

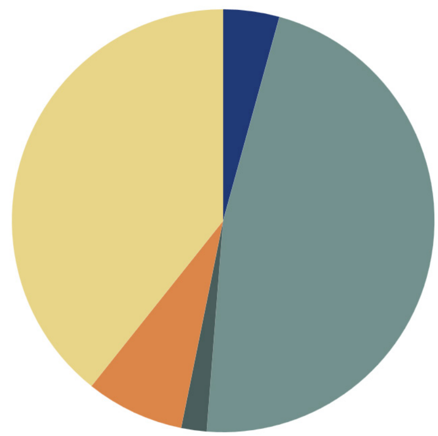
Investment Portfolio

LDRD investments span a broad range of research topics, helping to ensure that LLNL supports innovation in key programmatic areas. Funded projects address some of our newest mission spaces, including cognitive simulation, predictive biology, space science and security, and hypersonic science. We also invest in the core capabilities and programmatic areas that undergird our Laboratory's technical vitality and mission agility.

For fiscal year 2024, we carefully structured Livermore's LDRD investment portfolio to promote the short-term objectives and long-term goals of DOE, NNSA, and our Laboratory. The key metrics presented here regarding our FY24 investment portfolio reflect this structure, including how funds are distributed across the program's 5 types of projects and 18 research categories. By strategically selecting the types of projects we fund, along with the amount of funding invested in each project, we help ensure a strong program portfolio.

FY24 INVESTMENTS
258 PROJECTS,
~$176M TOTAL FUNDING

Percentage of Funding by Category



Exploratory Research	47%
Strategic Initiative	39%
Lab-wide Competition	8%
Disruptive Research	4%
Feasibility Study	2%

Funding by Project Type

Livermore's LDRD program includes five types of projects. Each one has a distinctive purpose, duration, and funding limit. For example, our one-year feasibility studies support relatively brief investigations of a specific technical approach. These types of projects can be launched mid-year to rapidly respond to an emerging challenge. Other types of projects span several years, often involving collaborators and research that tackles a broader scope of challenges.

Project Type	FY24 Projects Funded	Project Aim
Exploratory Research	150	Address a specific research challenge or enhance a core competency.
Feasibility Study	34	Determine the viability of a new way to address a mission-relevant challenge.
Lab-wide Competition	43	Conduct innovative basic research and enable out-of-the-box thinking.
Strategic Initiative	22	Make significant progress addressing a mission-relevant challenge from a multidisciplinary perspective.
Disruptive Research	9	Pursue novel ideas with the potential to overturn fundamental paradigms or create new research directions.

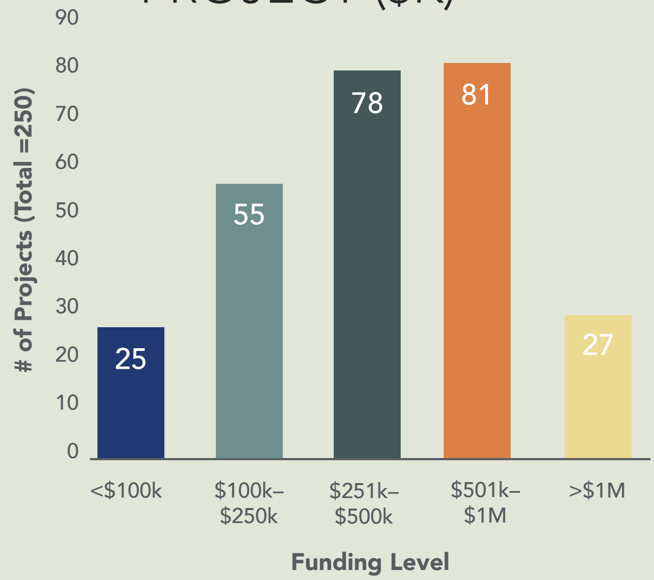
Projects by Funding Level

Our Laboratory's investment strategy includes the flexibility to fund projects at varying dollar amounts, depending on the project scope. This chart presents data on the number of projects funded in FY24, distributed across five funding levels. The largest number of projects (95) fell in a higher funding range, receiving between 501k and 1000k per project. A smaller number of projects received less than $100k in funding (17 projects), or more than $1M in funding (26 projects).

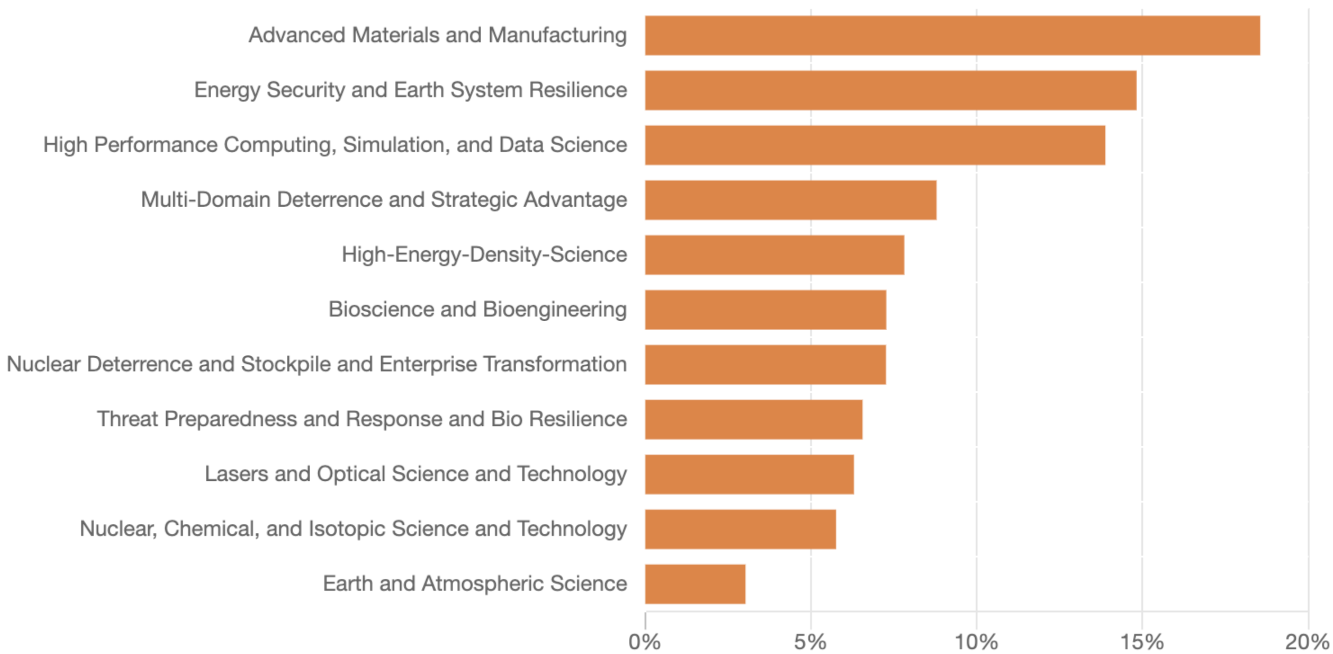
Funding by Research Area

Every LDRD project is assigned to at least one of the Laboratory's research areas in the LDRD investment portfolio. The categories include 11 mission-driven research challenges and 7 core competencies—capabilities that enable us to conduct high-priority, mission-relevant research. (Note that this chart only includes research categories where at least one project designated the category as a primary research focus.)

$682,000 AVERAGE FUNDING LEVEL PER PROJECT ($K)



Percentage of Project Cost by Research Category



Program Value

From publications to intellectual property to long-term impact, LDRD is a major contributor to the Laboratory's scientific and technological accomplishments.

75 INSTITUTIONS were involved in formal collaborations with LLNL as part of LDRD-funded research teams in FY24.

Collaborative Explorations

External collaborations are essential to the innovative research that takes place at LLNL, including LDRD-funded projects. By collaborating with other national laboratories, academia, and industry, our investigators can engage with experts from other institutions and access world-class experimental facilities.

The following table provides our most recent data regarding formal collaborations, which we define as LDRD-funded projects where an external collaborator received LDRD funds from LLNL. In addition, our investigators frequently participate in informal collaborations with researchers at other institutions, which often involve joint scientific publications. Both types of collaborations are a key indicator of the broad intellectual engagement that is a hallmark of LLNL's research environment.

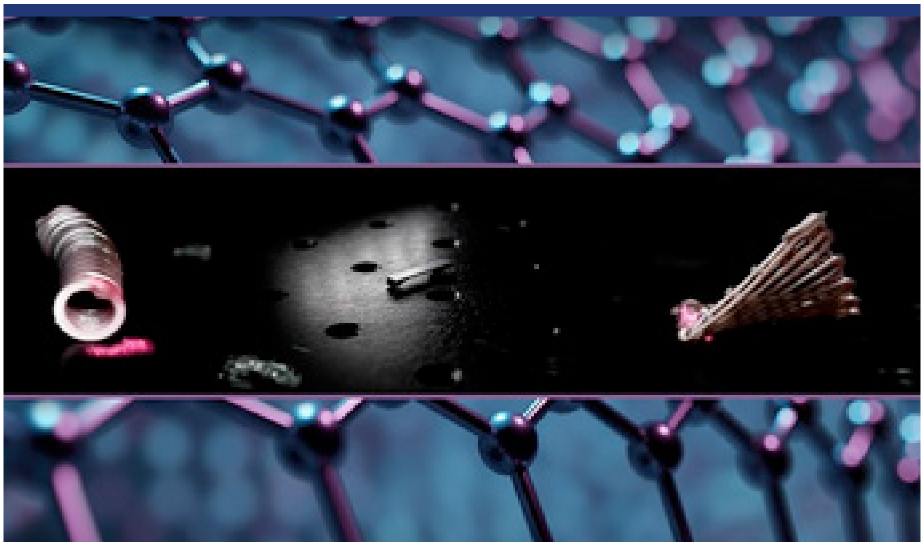
Collaborations	FY20	FY21	FY22	FY23	FY24
LDRD-funded projects with one or more formal collaborations	78	88	79	81	79
Percentage of LDRD projects	32%	33%	32%	30%	31%

Are shapeshifting "soft machines" in our future? LLNL scientists advance light-responsive material

Researchers at Lawrence Livermore National Laboratory have furthered a new type of soft material that can change shape in response to light, a discovery that could advance "soft machines" for a variety of fields, from robotics to medicine.

The novel material, called a liquid crystal elastomer (LCE), is made by incorporating liquid crystals into the molecular structure of a stretchable material. Adding gold nanorods to the LCE material, scientists and engineers created photo-responsive inks and 3D printed structures that could be made to bend, crawl and move when exposed to a laser that causes localized heating in the material. The results were recently published online by Matter, and will be featured in the journal's March 2025 print issue.

The LLNL team, along with their collaborators from Harvard University, North Carolina State University and the University of Pennsylvania, used a direct ink writing printing technique to build a variety of light-responsive objects, including cylinders that could roll, asymmetric "crawlers" that



Lawrence Livermore National Laboratory researchers and their collaborators have created a new responsive material called a liquid crystal elastomer, made by incorporating liquid crystals into the molecular structure of a stretchable material. Adding gold nanorods to the material, the researchers created photo-responsive inks and 3D printed structures that could be made to bend, crawl and move when exposed to a laser light. (Photos courtesy: Michael Ford)

Principal Investigator: Caitlyn Krikorian Cook

LDRD Project: 22-ERD-030 Shape Changing of Responsive Elastomer Structures

could go forward and lattice structures that oscillated. By combining shape morphing with photoresponsivity, researchers said the new type of material could change the way people think about machines and materials.

"At LLNL, we've focused on developing static materials and architectures for some time," said principal investigator Caitlyn Krikorian (Cook). "We've made these complex types of structures like hierarchical lattices, and we've even started exploring more responsive materials, like shape memory polymers, that have a one-time shape memory response. But the Lab really hadn't delved deep into creating architectures that can go from a 3D-to-3D type of shape change. This project is starting to show how architecture and these novel materials can have unique modes of actuation that we haven't researched before."

Researchers said the new material could be used to create a "soft machine" — a type of machine made from these flexible LCE composite materials — capable of responding to external stimuli and even mimicking the movements and behaviors of living organisms. Soft robots made of the shape-morphing material could crawl, swim or fly, and explore environments that are too difficult or dangerous for humans to access, like caves or outer space. Soft machines could also be used in medical applications, such as implantable devices that can adapt to the body's movements, or prosthetic limbs that move like natural limbs, and other applications that aren't possible with machines made from rigid materials, like metal or plastic.

Researchers said the movement of the LCE material is driven primarily by a process known as photothermal actuation, which involves converting light energy into thermal energy resulting in a mechanical response from the material. Driven by the interaction between light, gold nanorods and the LCE matrix, the process enables the printed structures to exhibit dynamic and reversible movements in response to external stimuli.

“When you have this composite material — in this in case, these gold nanorods in these liquid-crystal elastomers — it has a photothermal effect,” Cook explained. “With [infrared] light, it creates a heating effect, which causes the aligned molecules to become misaligned. During that misalignment process, if there’s uniform heating, you’ll have a global shape change. But in this case, we can have localized heat change, which is how you can get those localized regions of shape morphing to do things like locomotion.”

In the study, researchers used a computer vision system, involving cameras and a tracking software, to control the movement of a printed cylinder. The tracking system monitored the position of the rolling cylinder and continuously adjusted the position of the laser to raster the edge of the cylinder. This continuous tracking and adjustment allowed the cylinder to maintain its rolling motion in a controlled manner.

By leveraging computer vision with the photothermal actuation of the cylinder, the researchers achieved a sophisticated level of manipulation of the soft machine’s movement, showcasing the potential for advanced control systems in the field of soft robotics and soft machines. The team also showed that responsivity could be controlled so the soft machines could perform useful tasks, such as a moving cylinder carrying a wire.

“[Lead author Ford] did some awesome work in using computer vision to control the locomotion of the printed cylinder and using a rastering laser to force it to move,” said co-author Elaine Lee. “But once you start to get into much more complex motion — like using various rastering speeds and light intensities on a printed lattice, causing it to move in various different modes — those were actually outside of what our high performance computing (HPC) simulations were able to predict, because those codes are expecting a uniform heating or stimuli on that lattice. So, using computer vision and machine learning to learn the actuation speeds, and what doses of light can cause locomotion from that printed architecture, will push us a lot further in understanding how our materials will respond.”

Researchers said there are still some challenges that need to be overcome before the material can be used in practical applications. The team found that structures they created could flip over or exhibit other unpredictable motion, thereby making it difficult to design specific modes of motions. They said they will continue to work on models that can describe the complex motion to better design future machines and develop new materials and manufacturing techniques to create soft machines that are more durable, reliable and efficient for a variety of applications. New control systems and computer algorithms also could enable soft machines to move and interact with their environment in a more intelligent and autonomous way, they said.

Cook said the team is looking at incorporating responses to different types of stimuli, beyond thermal and light stimuli, into areas like humidity and energy absorption, and conditions that the material might experience in space. She added that the team is looking at starting a new Strategic Initiative at the Lab to focus on autonomous materials and “move the needle” towards sentient materials.

“We’re all thinking about ways to make materials more autonomous; sentient materials that can sense, respond, be programmed, learn, decide and communicate," Cook said. "These liquid crystal elastomers are responsive materials — they're able to sense a stimuli and respond and will respond repeatedly every time — but it doesn't have a sense of memory or a way to learn the repeated stimuli and respond accordingly. It doesn't have a means to communicate yet, other than potentially being able to pair it with some type of mechanical computing. These are really the materials that we're striving towards, and this might be a five- to 10-year timespan of effort."

Intellectual Property

Year after year, projects sponsored by LDRD achieve a disproportionately large percentage of the patents and copyrights issued for LLNL research. As illustrated in the following tables, LDRD-funded work has been key in developing more than half of the Laboratory's patents, one-third of the Laboratory's copyrights (chiefly computer code), and more than half of the Laboratory's records of invention.

LDRD-funded work has played a key role in developing

MORE THAN 50%

of the Laboratory's patents.

Patents	FY20	FY21	FY22	FY23	FY24
All LLNL patents issued	200	166	166	197	200
LDRD patents issued	131	96	103	116	126
LDRD patents as a percentage of total	66%	58%	62%	58%	63%

Copyrights	FY20	FY21	FY22	FY23	FY24
All LLNL copyrights	138	125	142	166	201
LDRD copyrights	31	42	47	44	66
LDRD copyrights as a percentage of total	22%	34%	33%	26%	33%

Records of Invention	FY20	FY21	FY22	FY23	FY24
All LLNL records	126	89	70	120	119
LDRD records	56	53	40	64	61
LDRD records as a percentage of total	44%	60%	57%	53%	51%

Elizabeth Grace (LLNL, right) and Filip Grepl (ELI Beamlines, left) assemble the PROBIES diagnostic, one of many instruments that fed data to the machine-learning optimizer algorithm. (Photo: Isabella Pagano/LLNL)

Principal Investigator: Matthew Hill

LDRD Project: 24-ERD-041 Autonomous Laser Optimization for High-Repetition-Rate Applications

Machine learning optimizes high-power laser experiments

Commercial fusion energy plants and advanced compact radiation sources may rely on high-intensity high-repetition rate lasers, capable of firing multiple times per second, but humans could be a limiting factor in reacting to changes at these shot rates.

Applying advanced computing to this problem, a team of international scientists from Lawrence Livermore National Laboratory (LLNL), Fraunhofer Institute for Laser Technology (ILT) and the Extreme Light Infrastructure (ELI ERIC) collaborated on an experiment to optimize a high-intensity, high-repetition-rate laser using machine learning.

"Our goal was to demonstrate robust diagnosis of laser-accelerated ions and electrons from solid targets at a high intensity and repetition rate," said LLNL's Matthew Hill, the lead researcher. "Supported by rapid feedback from a machine-learning optimization algorithm to the laser front end, it was possible to maximize the total ion yield of the system."

The researchers trained a closed-loop machine learning code developed by LLNL's Cognitive Simulation team on laser-target interaction data to optimize the laser pulse shape, allowing it to make adjustments as the experiment ran. Data generated during the experiment was fed back into the machine learning-based optimizer, allowing it to tweak the pulse shape on the fly.

The laser fired every 5 seconds, consistently exceeding laser intensities of $3x10^{21}$ W/cm^2 its focus, stopping after 120 shots when the copper target foil had to be replaced. During this time, the researchers also inspected the diagnostics for damage and assessed debris accumulation from vaporized targets. The team conducted experiments at ELI for three weeks, with experimental runs lasting approximately 12 hours per day, during which the laser would fire up to 500 shots.

The experiment took place at the ELI Beamlines Facility in the Czech Republic, where the researchers utilized the state-of-the-art High-Repetition-Rate Advanced Petawatt Laser System (L3-HAPLS) to generate protons in the ELIMAIA laser-plasma ion accelerator. Focusing on the goal of applying machine learning to a high-rate-laser experiment, the team simplified aspects of the experiment as much as possible, like using a robust, simple copper foil target.

"By harnessing the HAPLS and pioneering machine learning techniques, we embarked on a remarkable endeavor to further comprehend the intricate physics of laser-plasma interactions," said Constantin Haefner, managing director of Fraunhofer ILT.

More than 4,000 shots were fired during the campaign, allowing statistical analysis to be performed on the results and demonstrating optimization of ion yield above the already-impressive nominal baseline performance.

Using machine learning was a new experience for the experimental physicists. "It becomes a spectator sport," Hill said. "We watched the data coming in and tried to guess what the optimizer would do. It's very different than an experiment with manual intervention."

LLNL becomes a L3-HAPLS user

The L3-HAPLS laser has excellent laser performance repeatability, displaying exceptionally stable alignment, focal spot quality and the ability to generate intense laser pulses at a high repetition rate to drive the generation of secondary sources such as electrons, ions and x-rays.

"The successful execution of such a complex experiment showcases the cutting-edge quality and reliability of the L3-HAPLS laser system," said Bedrich Rus, chief laser scientist at ELI Beamlines.

LLNL developed the HAPLS laser as part of a bilateral agreement with ELI Beamlines, with first light from the system after delivery and installation in the Czech Republic in 2017. This was only the second user experiment at the facility, having been awarded time through a competitive worldwide call for proposals, now issued twice annually and attracting hundreds of applications.

Lengthy preparation pays off

In addition to Hill, the LLNL team of Elizabeth Grace, Franziska Treffert, James McLoughlin, Isabella Pagano, Abhik Sarkar, Raspberry Simpson, Blagoje Djordjevic, Matthew Selwood, Derek Mariscal, Jackson Williams and Tammy Ma spent about a year preparing for the experiment with the Fraunhofer ILT and ELI Beamlines teams. In addition to local facility diagnostics, the Livermore team fielded several instruments developed under the Laboratory Directed Research and Development Program, including the REPPS magnetic spectrometer, PROBIES ion beam imaging spectrometer, a rep-rated scintillator imaging system and rep-rated X-ray spectrometer.

An international team from LLNL, Fraunhofer Institute for Laser Technology and the Extreme Light Infrastructure collaborated to use machine learning to optimize experiments on the L3-HAPLS laser. (Photo courtesy: Eli Eric)

To follow export control regulations, the machine learning code had to be run at LLNL to segregate it from computer systems at ELI Beamlines. This created a challenge of rapidly transferring data between the Czech Republic to LLNL to keep pace with the laser.

Sarkar helped engineer the trans-Atlantic coupling between computers at LLNL and at ELI for real-time closed-loop operation. “Thanks to hard work on both sides, we came up with a solution,” he said. “On the computing side, this opens up new possibilities for remote operation.”

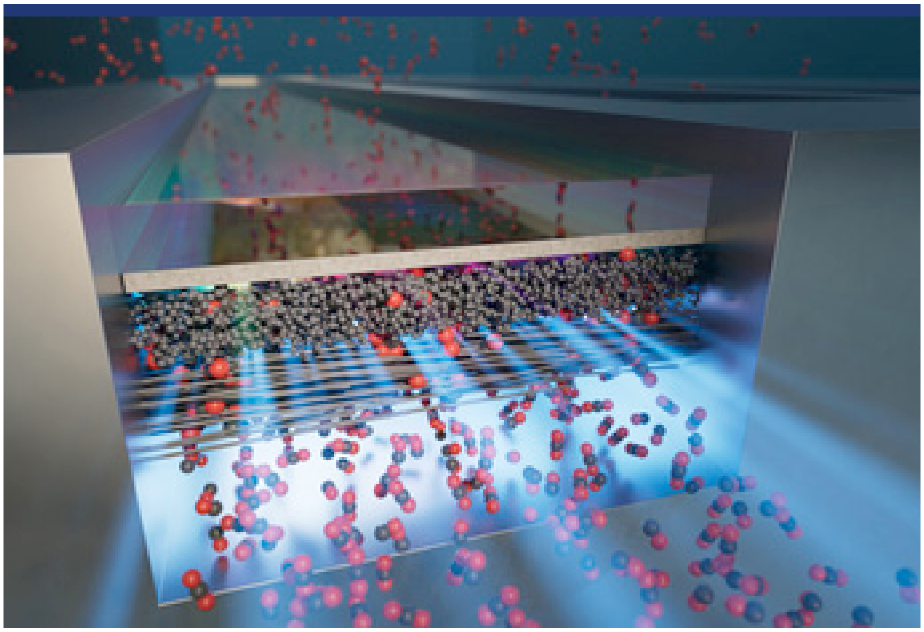
The experiment was very successful, generating robust data from the first day. In future experiments, the team hopes to allow machine learning to control additional parameters like the focal spot and to use the approach at different experimental facilities.

More broadly, the success of coupling state-of-the-art laser technology with machine learning techniques could open new avenues for advancements in various fields such as fusion energy, medical therapy, materials science and non-destructive analysis in the field of cultural heritage and archaeology.

Scientific Publications

Laboratory scientists and engineers publish more than a thousand papers each year in a wide range of peer-reviewed journals, of which LDRD-funded work accounts for a large portion. The numerous publications made possible through LDRD-sponsored research help the Laboratory maintain a strong presence in the broader scientific community, extending the impact of LDRD research beyond the DOE mission space into the wider scientific arena. In addition, the impact of these publications documenting LDRD project results extends long after articles appear in the journals, increasing the value of LDRD investments in these projects.

Journal Articles	FY20	FY21	FY22	FY23	FY24
All LLNL articles	1,149	1,256	1,149	1,218	1,004
LDRD articles	428	509	490	495	409
LDRD articles as a percentage of total	37%	41%	43%	41%	41%



The front cover of 'ChemElectroChem' shows a membrane electrode assembly performing CO2 electrolysis, where the CO2 flows through the device and undergoes a series of chemical reactions before exiting in the form of carbon monoxide.

Modeling CO_2 electrolysis

LLNL researchers and collaborators are working under a Laboratory Directed Research and Development-funded initiative (22-SI-006) to design next-generation electrochemical reactors for industrial CO_2 conversion using computationally driven algorithms.

These electrolyzers can produce mixtures of different carbon-based products depending on the catalyst used. Copper catalysts, for example, can produce ethylene — the most common carbon-based commodity chemical in the world. It is the key component in a myriad of household and construction products from water bottles, carpeting, and toys to pipes, insulation, and many more.

Silver catalysts, on the other hand, can produce carbon monoxide and hydrogen, a mixture known as syngas, which is commonly used to make fuels and chemicals. In one study, published on the cover of *ChemElectroChem,*

Principal Investigator: Sarah Baker

LDRD Project: 22-SI-006 The Science of Scale-Up: Accelerated Scaling of Materials and Manufacturing Solutions

LLNL researchers developed Multiphysics models for two different designs — a zero-gap membrane electrode assembly (MEA) and a planar electrode with silver catalysts.

Historically, MEA electrolyzers (the device that is used to electrically transform the CO_2 to produce products like ethylene and syngas) have offered significantly improved performance due to their "zero-gap" design. However, they have also been known to accumulate liquid in porous regions of the cell, a phenomenon known as flooding, which slows down the reaction rate and decreases the efficiency of the electrolyzer.

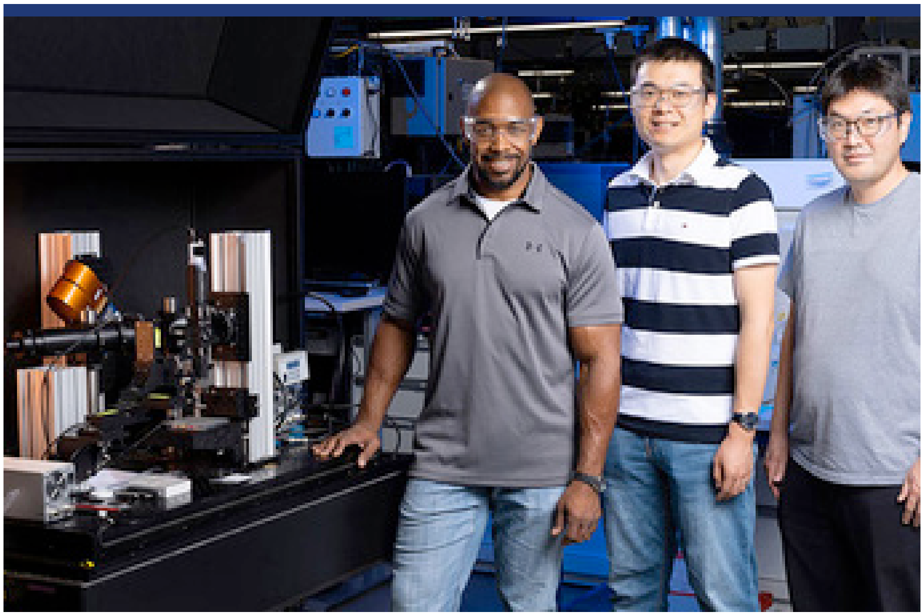
The team's research is helping to evaluate the pros and cons of these different electrochemical conversion solutions, helping them to understand the factors associated with these limitations as they work to build an end-to-end model that simulates CO_2 mass transfer across an industrialized reactor from start to finish. With this model, the researchers can optimize the reactor by simulating how different "ingredients" (catalyst used, device design, etc.) affect the CO_2 conversion process.

Early Career Opportunities: Students and Postdoctoral Fellows

By funding exciting, potentially high-payoff projects at the frontiers of science, the LDRD program attracts top talent in new and emerging fields of science and technology. As shown in the following tables, LDRD investments contribute to the health and robustness of LLNL's student and postdoctoral researcher programs.

Students	FY20	FY21	FY22	FY23	FY24
Students supported by LDRD	101	136	149	185	216
Percentage of all students	18%	24%	23%	24%	26%

Postdoctoral Researchers	FY20	FY21	FY22	FY23	FY24
Postdoctoral researchers supported by LDRD ≥10% of their time	208	208	240	213	234
Percentage of all postdoctoral researchers	63%	54%	56%	51%	58%
LDRD postdoctoral researchers converted to full staff	60	50	72	56	44
Percentage of all conversions	77%	82%	77%	70%	66%



From left, Marcus Worsley, Longsheng Feng and Tae Wook Heo have created a new electrode that that will help increase storage capacity. (Photo: Blaise Dorous/LLNL).

3D-printed electrode is all charged up

The architectural design of electrodes offers new opportunities for next-generation electrochemical energy storage devices (EESDs) by increasing surface area, thickness and storage capacity.

But conventional thick electrodes increase ion diffusion length and cause larger ion-concentration gradients, limiting reaction kinetics, including storage capacity.

To overcome these challenges, Lawrence Livermore National Laboratory (LLNL) scientists and collaborators at the University of California, Santa Cruz 3D-printed a new and compact device configuration with two interpenetrated, individually addressable electrodes, allowing precise control over the geometric features and interactions between the electrodes.

Using powerful high-performance computing facilities at LLNL, the team

Principal Investigator: Marcus Worsley

LDRD Project: 23-SI-002 Advanced Energy Storage Technologies for Extreme Conditions demonstrated through computational simulation that the interpenetrated electrode design improves ion-diffusion kinetics in EESDs by shortening the ion-diffusion length and reducing ion-concentration inhomogeneity.

"The device with interpenetrated electrodes outperformed the traditional separate electrode configuration, enhancing both volumetric energy density and capacity retention rate," said LLNL postdoc Longsheng Feng, co-author of a paper appearing in Nano-Micro Letters. This free-standing device structure also avoids short-circuiting without needing a separator. The feature size and number of interpenetrated units can be adjusted during printing to balance surface area and ion diffusion. The team used a zinc manganese dioxide battery as a model system and found that the device outperforms conventional separate electrode configurations, improving volumetric energy density by 221% and exhibiting a higher capacity retention rate of 49% compared to 35% at temperatures from 20 to 0 °C.

"Our study introduces a new EESD architecture applicable to lithium-ion, sodium-ion batteries, supercapacitors and other storage systems," Feng said. "To our knowledge, this is the first time that interpenetrated lattices have been used for architectural EESDs."

Significantly ordered, periodically entangled two electrodes occupying the same free volume are close to each other throughout the whole structure regardless of its thickness. This structural characteristic is anticipated to enhance the ion diffusion kinetics during the charging and discharging processes.

"This new tool kit of materials and designs will enable high-performance energy storage in conditions relevant to national security missions and the broader energy storage community," said LLNL scientist Marcus Worsley, a co-lead author.

Other LLNL authors include Tae Wook Hoo and Cheng Zhu.

Professional Fellows

APS physics™

One relevant indicator of advancement and leadership in a scientific field is the election of individuals as fellows of professional societies. This indicator reflects success for both the individual researcher and the Laboratory as a whole.

American Physical Society (APS) fellowships are awarded based on scientific merit and impact over an extended period, and the evaluation process relies on nomination and recommendation by peers. As such, data regarding the history of APS fellowships awarded to LLNL physicists provide an important indicator regarding the key role that the LDRD Program plays in developing the technical, scientific, and leadership skills of early career staff. As presented in the following table, for fiscal year 2023, 100% of the new APS Fellows from LLNL have early career LDRD experience.

Because the quantity of awards each year is a small number, we also present multi-year statistics. For example, over the last 20 years, more than 90% of the APS Fellows at LLNL had early career LDRD experience.

TRACING IMPACT TO LDRD ROOTS

Throughout this section, we mention "LDRD roots." Much discussion with principal investigators has transpired about what it means for an accomplishment to have LDRD roots. A simple case would be if an idea for an invention arises during an LDRD project and work on the invention is completed during the period of LDRD investment. But R&D often does not advance on such a short timescale. In general, an accomplishment (invention, paper, capability, etc.) is determined to have LDRD roots if at least one LDRD project needed to occur for the accomplishment to take place. In other words, if one can identify an LDRD project that was critical to the accomplishment, then it is considered to have LDRD roots. Two LLNL scientists were selected as 2023 fellows of the American Physical Society. The new fellows were both selected by the APS Division of Plasma Physics.

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

HISTORY OF APS FELLOWS AT LLNL

	FY22	FY23	FY23	FY15–19	FY20–24	FY15–24
Total APS awards	2	2	3	24	14	38
Awards with LDRD roots	2	2	3	23	14	37
% with LDRD roots	100%	100%	100%	96%	100%	97%
Average years from first LDRD experience	15	15.5	8.3	15.6	13	14.6

2024 APS Fellows at LLNL
Three Lab scientists named 2024 APS Fellows

Lawrence Livermore National Laboratory (LLNL) scientists Daniel Casey, Daniel Clark and Raymond Smith have been named 2024 American Physical Society (APS) Fellows.

Casey was selected for "outstanding contributions to the understanding of the stagnation conditions required to achieve ignition." Clark was honored for "extensive contributions to inertial confinement fusion state-of-the-art implosion modeling, innovative ignition designs, novel applications of laser-plasma interactions, and the scientific understanding of hydrodynamic instabilities." Smith was selected for "for pioneering dynamic ramp-compression experiments on high-energy laser facilities, resulting in significant discoveries in high-pressure materials physics and planetary science."

The APS Fellowship Program was created to recognize members who may have made advances in physics through original research and publication or made significant innovative contributions in the application of physics to science and technology. They also may have made significant contributions to the teaching of physics or service and participation in the activities of the society.

Fellowship is a distinct honor signifying recognition by one's professional peers. Each year, no more than one half of one percent of the society's membership (excluding student members) is recognized by their peers for election to the status of fellow of the American Physical Society. "This new tool kit of materials and designs will enable high-performance energy storage in conditions relevant to national security missions and the broader energy storage community," said LLNL scientist Marcus Worsley, a co-lead author.

APS Fellow

2024 APS Fellows at LLNL

DANIEL CASEY
Experimental excellence in fusion research

"I am humbled and incredibly honored to be named an APS Fellow," he said. "It is often said that scientists stand on the shoulders of giants. Indeed, I am indebted to my friends and colleagues who have helped me at every stage of my research and am deeply grateful."

Daniel Casey is a physicist who works in the National Ignition Facility (NIF) and Photon Science Directorate and is the low mode working group lead for the Inertial Confinement Fusion (ICF) program. He was recently appointed group leader for the Implosions & Stagnations (Hydrodynamics) group. His work focuses on diagnosing and assessing the impact of asymmetries in ICF implosions.

DANIEL CLARK
Leading the charge in ICF design and modeling

"To join so many of my exceptional colleagues in the ICF program in receiving the APS Fellowship is a profound honor," Clark said. "The recognition not only acknowledges my individual contributions to the field but also highlights the Laboratory's collaborative efforts. This honor inspires me to continue our pursuit of groundbreaking advancements in plasma physics."

Daniel Clark is a physicist who works in the Strategic Deterrence Directorate at LLNL and specializes in ICF design and modeling. He has served as the design lead for several experimental campaigns at NIF and, from 2013 to 2021, led the capsule modeling working group within the ICF program.

RAYMOND SMITH
Pioneering dynamic ramp-compression techniques

"I'm honored to be selected as an APS Fellow, and I deeply appreciate this recognition from the American Physical Society. This distinction reflects the collaborative efforts of my colleagues, mentors and students who have contributed to my research journey. It motivates me to continue pushing the boundaries of scientific discovery and to foster a spirit of curiosity and innovation within the broader physics community," Smith said."

Raymond Smith is a physicist who works in the Physical and Life Sciences Directorate and is the lead principal investigator for the NIF TARDIS X-ray diffraction platform, which has provided direct measurements of crystal structure and microstructural texture at terapascal (TPa) pressures (1 TPa is equivalent to 10 million Earth atmospheres).

Long-term Impact

The LDRD program is an investment in our nation's future, ensuring mission support that is often realized many years after an LDRD-funded project concludes. Recognizing this long-term impact of the LDRD program, we believe it is important to highlight indicators that span multiple years, demonstrating the true impact of LDRD as a national asset.

We collaborated with our colleagues from LDRD programs at other NNSA institutions to identify ways that we could best represent the long-term impact of LDRD investments. As each institution issues its LDRD program report for fiscal year 2024, we present a common set of long-term performance indicators including the content provided below.

Distinguished Member of the Technical Staff

One relevant indicator of career advancement in a science and technology field is the recognition of individuals as distinguished members of the technical staff at the institution. Individuals who receive this recognition are identified as being in the top 1% or 2% of the institution's scientific and technical staff, similar to a lifetime achievement award, or in this case, for their contribution to the Laboratory's mission.

At LLNL, appointment as a Distinguished Member of the Technical Staff (DMTS) is reserved for Laboratory scientists and engineers who have demonstrated a sustained history of high-level achievements in programs of importance to the Laboratory, become a recognized authority in the field, or made a fundamental and important discovery that has sustained, widespread impact.

As presented in the table, a vast majority of these distinguished staff at LLNL had early career experience with LDRD projects, which helped them develop their scientific, technical, and leadership skills.

HISTORY OF DMTS AWARDS AT LAWRENCE LIVERMORE NATIONAL LABORATORY

	FY22	FY23	FY24	FY15-19 (5 yrs)	FY20-24 (5 yrs)	FY15-24 (10 yrs)
Total DMTS awards	26	0	23	25	49	74
DMTS with LDRD roots	20	N/A	12	23	32	55
% with LDRD roots	77%	N/A	52%	92%	65%	74%
Average years from first LDRD experience	16.4	N/A	14.5	20.5	15.7	17.7

R&D 100 Awards

Another indicator of advancement and leadership in a scientific field is the R&D 100 Award program, which honors the top innovations of the past year. R&D 100 Awards can occur a long time after the initial ideas are developed, often during LDRD projects. Typically, it takes 5 to 10 years (or longer) from concept development to receiving an award, including the time needed to move through patenting an invention and demonstrating its commercial applications.

The LDRD program is an investment in our nation's future, ensuring mission support that is often realized many years after an LDRD-funded project concludes. Recognizing the is long-term impact of the LDRD program, we believe it is important to highlight indicators that span multiple years, demonstrating the true impact of LDRD as a national asset.

Over the last 10 years, **OVER 30% OF LLNL'S R&D 100 AWARDS** had roots in the LDRD Program.

HISTORY OF R&D 100 AWARDS AWARDS AT LAWRENCE LIVERMORE NATIONAL LABORATORY

	FY22	FY23	FY24	FY15-19 (5 yrs)	FY20-24 (5 yrs)	FY15-24 (10 yrs)
Total R&D 100 awards	3	3	3	17	13	30
Awards with LDRD roots	2	3	2	6	7	13
% with LDRD roots	67%	100%	67%	35%	54%	43%
Average years from first LDRD investment	7.5	14.7	13.5	7.3	12.3	10

Lab scientists win three R&D awards

Lawrence Livermore National Laboratory (LLNL) scientists and engineers have netted three awards among the top 100 inventions worldwide.

The trade journal *R&D World Magazine* recently announced the winners of the awards, often called the "Oscars of innovation," recognizing new commercial products, technologies and materials that are available for sale or license for their technological significance.

With this year's results, the Laboratory has now collected a total of 179 R&D 100 awards since 1978.

This year's LLNL R&D 100 awards include a software suite that helps apply deep-learning techniques to major science and data challenges in cancer research; software that helps better understand the power, energy and performance of supercomputers; and a number format that permits fast, accurate data compression for modern supercomputer applications.

"The R&D 100 awards highlight the most innovative, game-changing technologies, and it is wonderful to see LLNL teams being recognized," Kim Budil said. "Having three projects selected for this honor shows clearly the high degree of excellence and ingenuity our scientists and engineers bring to creating impactful solutions to important challenges."

The EXtreme-power, Ultra-low-loss, Dispersive Element (EXUDE) Elite optical element is one of three LLNL technologies awarded 2024 R&D 100 awards.

OPTICS BREAKTHROUGH IMPROVES LASER PERFORMANCE

Demand for high-power laser sources with diffraction-limited beam quality is increasing as material processing techniques such as marking, cutting, welding and drilling often require a laser beam that can transmit over distance while maintaining excellent quality, to minimize undesired beam spreading.

The increased demand is leading to a significant scaling effort for laser systems' output power to reach hundreds of kilowatts and even megawatts. However, challenges to scaling the output power include removing heat waste, maintaining beam quality and avoiding damage to output optics.

The EXUDE Optical Element Team: Mike Rushford, James Nissen, Hoang Nguyen, Candis Jackson, Sean Tardif and Brad Hickman.

The Extreme-power, Ultra-low-loss, Dispersive Element (EXUDE) Elite optical element addresses these challenges by concentrating light from multiple lasers with different wavelengths into a single, high-power beam with unparalleled compactness and damage-resistance.

EXUDE Elite significantly improves upon the original EXUDE technology (winner of a 2014 R&D 100 award), which made it possible to use Spectral Beam Combining (SBC) for near-diffraction-limited quality laser systems with first-ever output powers approaching megawatt levels. EXUDE Elite combines fiber laser beams via transmission through a fused silica optic, which is achieved in a less-expensive, more compact system with a 100-fold improvement to the damage threshold.

EXUDE Elite is a breakthrough that suggests a paradigm shift in high-power laser technology. The lower price and improved overall optics performance of EXUDE Elite offer the opportunity for wider access to SBC for industrial laser systems, ushering the laser power-scaling effort forward on a larger scale than ever before.

HIGH-PERFORMANCE MEMORY MAPPING LIBRARY

Supercomputing and high performance computing (HPC) are critical for enabling and accelerating scientific research. Accompanying the exponential growth in compute power is a complex and deep memory hierarchy, which creates inefficiencies when moving data from its storage

The team behind the R&D100 award winning technology UMap, a key solution for deep and complex memory and storage systems. The UMap team is led by LLNL computer scientist Maya Gokhale, a distinguished member of the technical staff (DMTS), and includes current team members Marty McFadden, Elena Green, Roger Pearce, Keita Iwabuchi and Karim Youssef and former Lab employee Ivy Peng.

Light refraction on full display from the EXUDE optical element location to the processor. Because of this, supercomputer applications face large, complex data problems from both the computer system (complex hierarchy, memory, and storage) and the application workload.

To address this, a team of LLNL computer scientists developed the UMap user-level library as part of the U.S. Department of Energy's Exascale Computing Project, specifically the Argo Project, in which UMap is a key solution for deep and complex memory and storage systems.

UMap offers a high-performance, application-configurable, unified memory-like interface to diverse datastores located across memory-storage hierarchical levels or even across a network. It is purpose-built for high performance through a highly optimized and configurable design and is recognized as a leading solution for memory mapping diverse and large datastores.

Freely available as open source, UMap is significantly aiding the scientific community and has been adopted in many high-impact scientific applications in industry, academia and national labs.

The LLNL part of the UnifyFS team is led by Lab computer scientist Kathryn Mohror, also a DMTS, and includes current team members Cameron Stanavige, Chen Wang, Hariharan Devarajan, Ned Bass and Tony Hutter, as well as former Lab employees Adam Moody and Danielle Sikich.

SPEEDING SIMULATION MODELING FOR IMPACT

UnifyFS, another R&D 100 award winner, was developed by a team from LLNL, Oak Ridge National Laboratory and the University of Illinois' National Center for Supercomputing Applications.

When HPC applications are used to simulate real-world phenomena, the results from predictive models can be used by policy makers to inform important, life-saving decisions. However, scientific simulations can take hours, days or even weeks to compute due to slowdowns in the dynamic input/output (I/O) communication between the supercomputer and the file.

The UnifyFS file system enables HPC science applications to perform I/O operations many times faster than they could with traditional methods.

UnifyFS is a temporary file system that uses fast storage tiers on supercomputers to quickly store and access application data, so that applications can produce their results in less time. In addition to providing high performance I/O operations, UnifyFS is easy to use and teams can leverage it without an administrator's help or changing their code to accommodate different types of HPC systems. Also available as open source and production-ready, UnifyFS makes I/O fast and easy so users can focus on their science.

UnifyFS collaborators are Lawrence Livermore and Oak Ridge National Laboratories, as well as the National Center for Supercomputing Applications at the University of Illinois.

LDRD's Long-Term Program Impact

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

As part of the Lawrence Livermore National Laboratory LDRD Annual Report, each year we include a chart showcasing the long-term impact of LDRD on the LLNL Missions and Science and Technology capabilities. This year we highlight LLNL's activities to innovate the next generation laser science at

R&D Challenge

Developing new laser materials and technologies to take advantage of improved laser material properties is a highly interdisciplinary endeavor, requiring expertise in:

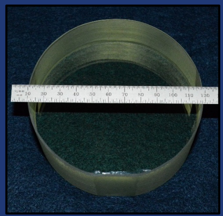
- Materials science (optical materials, crystals, multi-layer coatings)
- Lasers / optical science (laser system design)
- Solid-state physics (laser diode pumping)
- Electrical engineering (pulsed power, detectors and diagnostics)
- Mechanical engineering (vacuum and thermal systems, optomechanics, structural analysis, CFD, etc.)

Approach

- Execute targeted component and technology R&D that reduces risks for a new integrated laser system build
- DARPA engagement to advance TRL of technologies for National Security applications
- Deploy a system to LLNL's Jupiter Laser Facility to enhance experimental capabilities for HED science
- NNSA programmatic funding for developing and demonstrating radiography and laser-material interaction (LMI) platforms
- Exploring use for enhanced efficiency in Extreme-UV lithography (EUVL)

2017 — *LDRD project rediscovers a laser gain medium with attractive material properties*

2019 — *Disruptive Research LDRD Funded, targets cost-effective single shot high laser pulse energy*

2021 — 

World record laser pulse energy at λ~2μm, 100× increase over state-of-the-art

2022 — U.S. Department of Energy, Office of Science — *HEP funds TechDev effort to demo avg power capability*

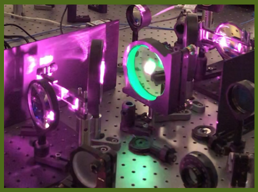
Lawrence Livermore National Laboratory | Los Alamos National Laboratory EST. 1943 | Sandia National Laboratories | Nevada National NNSS Security Site

LLNL. The lab has been a leader in laser materials and laser science since the laboratory was formed; over the last 10 years, seeded by the LDRD program, LLNL has created a new laser research and development ecosystem for high pulse energy short wave infrared (SWIR) lasers at ~2μm wavelength and their applications in national security and beyond. Focusing on advances in optical materials, laser diode pumping, and laser system design, LLNL has pushed the frontiers of laser technology in the ~2μm wavelength region to obtain a world record pulse energy (>100J) and world record peak powers (>1TW). These new capabilities are being studied and exploited for NNSA and National Security applications in radiography and for deeper understanding of important physics phenomena such as laser-material interactions. It also drives new research and development opportunities in extreme ultraviolet lithography (EUVL) as well as imaging and detection of nuclear materials and deeply buried geophysical structures.

Impact and Benefit

- External (non-NNSA) sponsors have invested ~$13M to-date, with ~$9M additional funds-in expected on currently-funded projects
- 2μm Related projects have trained/equipped 4 new PIs and an additional 4 new staff and PostDocs
- Within NNSA, this tech will enable new static and dynamic radiography capabilities for stockpile use (CT and NDE), and for LMI effects testing
- Multiple possible CRADA / SPP customers will likely leverage tech development for National Security and Competitiveness

2023 — *DARPA creates MuS2 program from seeing LDRD-funded capabilities*



2023 — *2μm Short-Pulse LDRD funded, component tech demonstrated, World Record λ~2μm peak power >1TW*

2024 — *MuS2 program demonstrates record laser-driven e-beam energy and muon generation for National Security apps*

2025 — *FES+BES CHIPS Act investment at LLNL to develop EUVL applications; HEP funds effort to develop mid-IR laser tech*

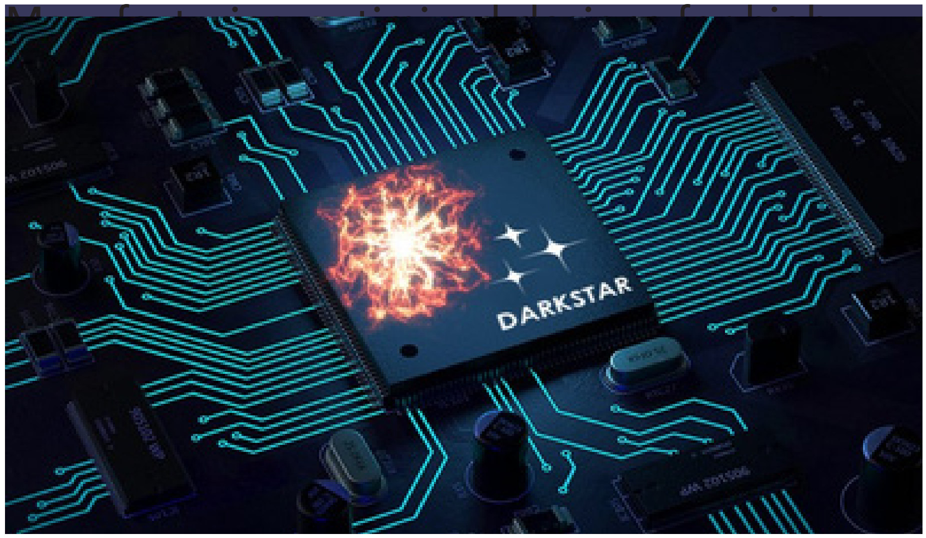
NNSA National Nuclear Security Administration

Program Accomplishments

LDRD-funded research explores the frontiers of science and technology in emerging mission spaces, with projects guided by an extremely creative, talented team of scientists and engineers.

Featured Research

LDRD funded 258 projects in the fiscal year 2024. Here, we provide a closer look at a handful of projects that underscore the exciting, innovative research in this year's LDRD portfolio. In addition, several PIs discuss their recent LRDR project experience in PI Perspectives.



LLNL researchers and collaborators observed a phase transition in magnesium oxide that Project DarkStar leverages artificial intelligence and machine learning to optimize shaped charges — explosive devices used to manipulate metals. (Image: Carol Le/LLNL and Adobe

When materials are subjected to extreme environments, they face the risk of mixing together. This mixing may result in hydrodynamic instabilities, yielding undesirable side effects. Such instabilities present a grand challenge across multiple disciplines, especially in astrophysics, combustion and shaped charges — a device used to focus the energy of a detonating explosive, thereby creating a high velocity jet that is capable of penetrating deep into metal, concrete or other target materials.

To address the challenges in controlling these instabilities, researchers at Lawrence Livermore National Laboratory (LLNL) are coupling computing capabilities and manufacturing methods to rapidly develop and experimentally validate modifications to a shaped charge. This work, published in the Journal of Applied Physics, is a part of Project DarkStar — a Laboratory Directed Research and Development-funded strategic initiative aimed at controlling material deformation by investigating the scientific problems of complex hydrodynamics, shockwave physics and energetic materials.

"Like a hurricane, shock waves and the detonation of explosives are typically deemed 'uncontrollable' events. But we have made it our goal to control these complicated dynamical systems," said DarkStar's principal investigator Jon Belof.

Principal Investigator: Jon Belof

LDRD Project: 21-SI-006 Project DarkStar: Controlling Material Deformation

The inspiration behind project DarkStar is deeply rooted in an unfinished line of research by Johnny von Neumann — a key member of the Manhattan Project and an expert in the nonlinear physics of hydrodynamics and shock waves. Having contributed to LLNL's world-leading reputation in computing, von Neumann is often considered the most gifted mathematician of his time.

Applying modern technologies to von Neumann's computational theories, the team employed artificial intelligence (AI) and machine learning (ML) to explore new, computationally optimized designs. The use of additive manufacturing — 3D printing — made it possible for researchers to rapidly realize even the most radical AI-designed components that would otherwise be considered "impossible" to create using traditional manufacturing methods.

To test their shaped charge designs — comprising a copper liner, a high explosive (HE) and a silicone buffer — the team conducted a total of 14 HE detonation experiments at LLNL's High Explosives Applications Facility from 2022 to 2023. These experiments compared a baseline design, which did not utilize a buffer between the liner and the HE, against a design with an optimized buffer to demonstrate the effectiveness of the silicone buffer as an instability mitigation technique.

"Each of our designs went through optimization, manufacturing and detonation testing in less than three months," said lead author Dylan Kline.

Once detonated, the metal liner is compressed and squeezed forward at about 5 kilometers per second, forming a high-velocity jet. The instability that this research aims to mitigate takes place when the explosive creates an impulse or "spike" at the materials interface, deforming and accelerating the metal (which has a high density) into the air around it (which has a low density). In this case, the instability or mixing of materials takes place when the jet forms in the air.

Kline said: "Our goal is to augment how this instability grows. If we can add something in our design to shape the shock waves, then we can control the way that energy is imparted on the metal liner."

Flash X-ray radiographs taken during the detonation experiments reveal the silicone buffer's ability to mitigate potential instabilities reliably and consistently.

Through their series of experiments, the team has uncovered several ground-breaking discoveries regarding hydrodynamic instabilities, including how to suppress an instability known as the Richtmyer–Meshkov Instability (RMI). RMI is of particular interest due to its unpredictable nature and role in materials undergoing extreme dynamic loading.

This research is directly applicable to aerospace engineering, as shaped charges are typically used for separating aircraft systems.

"This is just one case where having more powerful explosives and more effective ways of using them to manipulate metal could improve our industrial ecology," Belof said.

Project DarkStar illuminates the potential of AI/ML to support a wide range of national security missions.

Principal Investigators: Raymond Smith, and Joel Bernier

LDRD Project: 15-ERD-012, 15-ERD-014, 17-ERD-014, and 20-ERD-044

Kinetics of Incipient Stages of Phase Transitions and Uncertainty Quantification and Experimental Design Using a Quantitative Forward Model for Kinematic X-Ray Diffraction

Magnesium oxide undergoes dynamic transition when it comes to super-Earth exoplanets

Researchers from Lawrence Livermore National Laboratory (LLNL) and Johns Hopkins University have unlocked new secrets about the interiors of super-Earth exoplanets, potentially revolutionizing our understanding of these distant worlds.

The focus of this work, magnesium oxide (MgO), a crucial component of Earth's lower mantle, is believed to play a similar role in the mantles of massive rocky exoplanets. Known for its simple rock salt (B1) crystal structure and geophysical significance, MgO's behavior under extreme conditions has long intrigued scientists.

Super-Earths, planets with masses and radii larger than Earth but smaller than ice giants like Neptune, are often inferred to have compositions similar to terrestrial planets in our solar system. Given the extreme pressures and temperatures within their mantles, MgO is expected to transform from its B1 structure to a cesium chloride (B2) structure. This transformation significantly alters MgO's properties, including a dramatic decrease in viscosity, which can drastically affect the planet's internal dynamics.

To pinpoint the pressure at which this transition occurs, the LLNL team and collaborators devised a novel experimental platform. This platform combines laser-shock compression with simultaneous measurements of pressure, crystal structure, temperature, microstructural texture and density — an unprecedented approach.

Conducting 12 experiments at the Omega-EP laser facility at the University of Rochester's Laboratory for Laser Energetics, the scientists compressed MgO to ultra-high pressures of up to 634 GPa (6.34 million atmospheres) for several nanoseconds. Using a nanosecond X-ray source, they probed the atomic structure of MgO under these conditions. The results were striking: the B1 to B2 phase transition in MgO occurred within the 400-430 GPa pressure range at a scorching temperature of around 9,700 Kelvin. Beyond 470 GPa, B2-liquid coexistence was observed, with complete melting at 634 GPa.

"This study provides the first direct atomic-level and thermodynamic constraints of the pressure-temperature onset of the B1 to B2 phase transformation and represents the highest-temperature X-ray diffraction data ever recorded," said LLNL scientist Ray Smith, author of a paper published in Science Advances. "These data are an essential for developing accurate models of super-Earth interior processes."

The B1-B2 transition is a model for other structural phase transformations, attracting decades of theoretical research focused on the atomic pathways facilitating this change. Using a forward model to simulate X-ray diffraction conditions, the research team was able to clarify the mechanism of the B1-B2 transition in MgO.

"Our X-ray diffraction data provides direct measurements of atomic-level changes in MgO under shock compression and the first determination of a phase transition mechanism at deep mantle pressures of super-Earth exoplanets," said LLNL scientist Saransh Soderlind.

LLNL researchers and collaborators observed a phase transition in magnesium oxide that is believed to reside in the interiors of Super-Earths, planets with masses and radii larger than Earth but smaller than ice giants like Neptune. (Image: Adobe Stock)

Evaluating trust and safety of large language models

Principal Investigator: Bhavya Kalikhura

LDRD Project: 20-ERD-014

Safe and Trustworthy ML

Amid the skyrocketing popularity of large language models (LLMs), researchers at Lawrence Livermore National Laboratory are taking a closer look at how these artificial intelligence (AI) systems perform under measurable scrutiny. LLMs are generative AI tools trained on massive amounts of data in order to produce a text-based response to a query. This technology has the potential to accelerate scientific research in numerous ways, from cyber security applications to autonomous experiments. But even if a billion-parameter model has been trained on trillions of data points, can we still rely on its answer?

Two Livermore co-authored papers examining LLM trustworthiness — how a model uses data and makes decisions — were accepted to the 2024 International Conference on Machine Learning, one of the world's prominent AI/ML conferences.

"This technology has a lot of momentum, and we can make it better and safer," said Bhavya Kailkhura, who co-wrote both papers.

More effective models

Training on vast amounts of data isn't confirmation of a model's trustworthiness. For instance, biased or private information could pollute a training dataset, or a model may be unable to detect erroneous information in the user's query. And although LLMs have improved significantly as they have scaled up, smaller models can sometimes outperform larger ones. Ultimately, researchers are faced with the twin challenges of gauging trustworthiness and defining the standards for doing so.

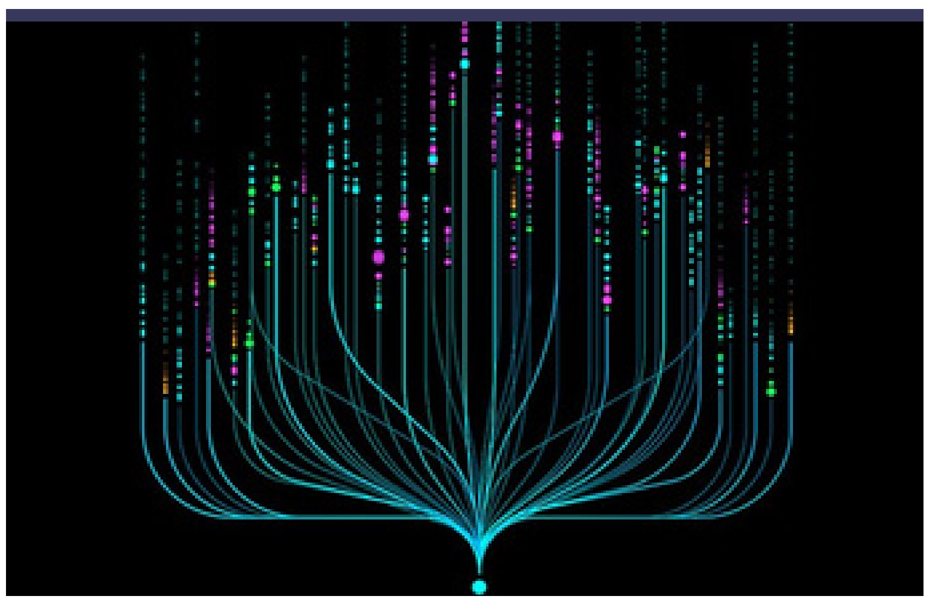
In “TrustLLM: Trustworthiness in Large Language Models,” Kailkhura joined collaborators from universities and research organizations around the world to develop a comprehensive trustworthiness evaluation framework. They examined 16 mainstream LLMs — ChatGPT, Vicuna, and Llama2 among them — across eight dimensions of trustworthiness, using 30 public datasets as benchmarks on a range of simple to complex tasks.

Led by Lehigh University, the study is a deep dive into what makes a model trustworthy. The authors gathered assessment metrics from the already extensive scientific literature on LLMs, reviewing more than 600 papers published during the past five years.

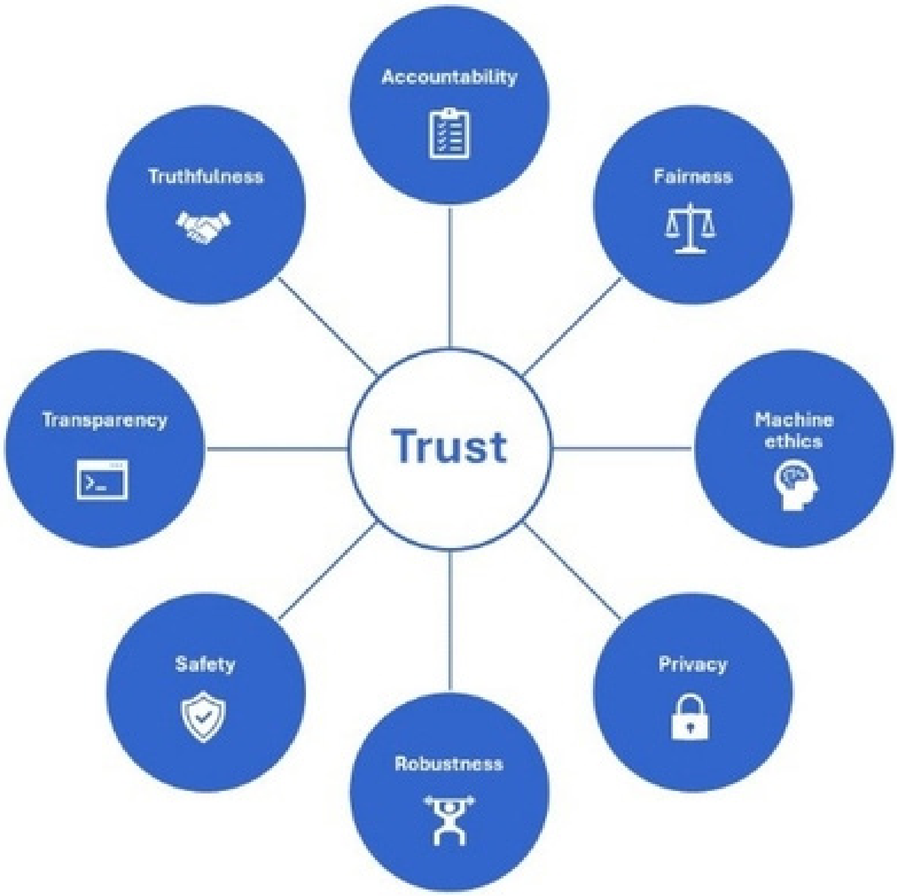
“This was a large-scale effort,” Kailkhura said “You cannot solve these problems on your own.”

The team’s resulting TrustLLM framework defines the following dimensions. A fair model avoids discriminatory outcomes, such as refusing to respond to demographic stereotypes or gender biases. Machine ethics measures a model’s recognition of human morals and emotions, such as discerning between right and wrong if a user’s query implies harming another person. Privacy measures whether a model reveals sensitive information even if the training dataset contains, for example, phone numbers.

Determining LLM trustworthiness requires assessment of how a model performs against tasks representing different dimensions of trust. See the Task & Dataset section of the study’s website for a list of datasets and the dimension(s) they correspond to. For example, a dataset used to test privacy leakage consists of half a million emails from the Enron Corporation. Others contain product reviews or medical diagnoses for synthetic patient records.



Additionally, robustness refers to a model’s ability to handle anomalies or unexpected data, and safety refers to its resilience against data manipulation or exploitation attempts, such as a request to provide ingredients for an explosive device. A truthful model presents facts, states its limitations —



such as if asked about a rapidly changing current event — and doesn't "hallucinate" inaccurate or nonsensical information.

Two other dimensions are more difficult to measure because of the complex, large-scale nature of LLMs. Accountability means providing the origin(s) of the output, while transparency refers to detailed explanations of decision-making steps and rationale.

These standards are high. As recent copyright-related headlines point out, LLMs don't cite their sources, nor do their owners assume responsibility for amalgamated datasets. Furthermore, training datasets can contain any number of imperfections, innocent or adversarial. A reasonably ethical model might be vulnerable to attacks.

"You can't look at one single aspect of trustworthiness. You have to look at how the model performs in all the metrics," Kailkhura said.

TrustLLM evaluations yielded mixed results. Most models refused to provide private information when instructed to follow a privacy policy, and answers to multiple-choice questions were more accurate than open-ended questions. Proprietary (closed-source) models tended to perform better than open-source models, which Kailkhura said could be attributed to companies' investments in development. Still, the best performing model in identifying stereotypes achieved only 65% accuracy, and performance across models varied considerably when faced with unexpected data. The team also noticed a trend of over-alignment, where models' safety scores are padded with false positives.

None of the tested models was truly trustworthy according to TrustLLM benchmarks. The good news, however, is that the study exposed where these models fail, which can encourage focus on trustworthiness as LLM developers continue to improve the technology.

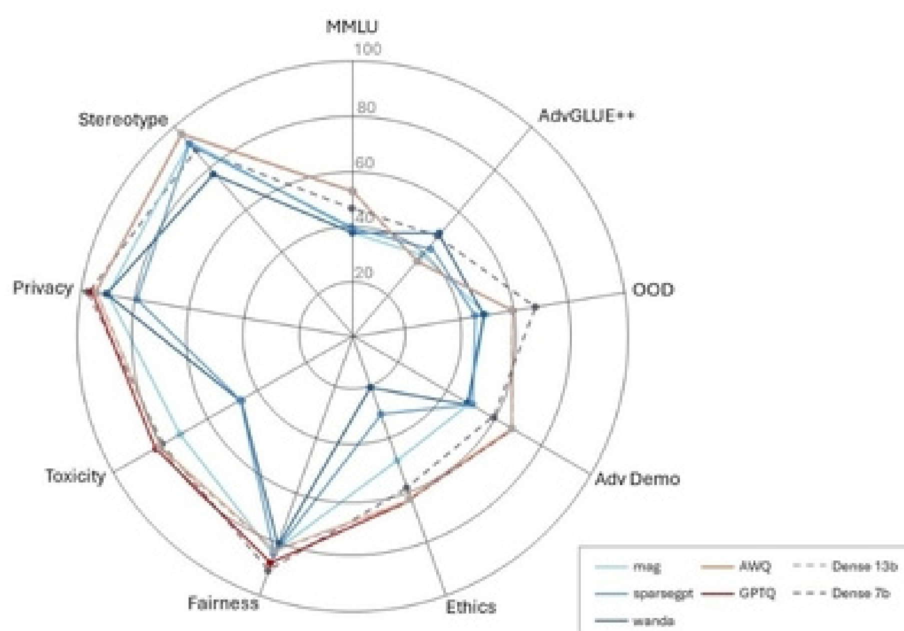
“LLMs are foundational models of increasing importance to the Lab and its national security applications, which is why our AI safety research is critical,” Kailkhura said.

More efficient models

As LLMs scale up, computational performance will continue to pose a challenge. Another conference paper investigates trustworthiness in the context of compression, where a model is modified to reduce the amount of data and compute resources necessary for efficiency. For example, compressing a model from 13 billion to 7 billion parameters can cut its latency in half, depending on the computing hardware running it. State-of-the-art compression techniques are designed to boost a model’s response speed, but they often prioritize performance over trustworthy results.

“Our research provides practical guidance for producing lightweight, trustworthy LLMs in research projects or applications throughout the Lab,” said James Diffenderfer, who co-authored “Decoding Compressed Trust: Scrutinizing the Trustworthiness of Efficient LLMs Under Compression” alongside Kailkhura, Brian Bartoldson and colleagues from several universities. The team applied five compression techniques to leading LLMs, testing the effects on various trustworthiness metrics.

This work builds on prior research in convolutional neural networks (CNNs) with compression techniques like pruning (removing nonessential parameters from the model) and quantization (reducing the model’s computational precision) — both of which can be applied to LLMs alone or in combination.



“Past Livermore research with CNNs showed that these techniques could affect accuracy and robustness,” Diffenderfer said. “To make LLMs more ubiquitous and usable through compression, it’s important to perform these studies and identify strategies to make LLMs more efficient without degrading their trustworthiness.”

The team discovered that compression via quantization was generally better — i.e., the model scored higher on trust metrics — than compression via pruning. Furthermore, they saw improved performance of 4-bit quantized models on certain trustworthiness tasks compared to models with 3- and 8-bit compression. Even at the same compression level, some models scored higher on ethics and fairness tasks and lower on privacy tasks, for instance.

Comparison of compressed (blue and orange solid lines) and uncompressed (dashed lines) LLMs across nine trustworthiness benchmarks, where a higher score indicates better performance. For example, GPTQ scores high in the benchmarks on the lower left side of the graph, but is weaker in the benchmarks on the upper right side.

“The effect on performance for each task varied based on the quantization algorithm used to compress the LLM,” Diffenderfer said. “Certain forms of compression are better suited for deploying lightweight LLMs without overly compromising their trustworthiness.”

In some cases, compression can even improve a model’s trustworthiness. Yet too much compression can backfire, as trustworthiness scores dropped after a certain point.

“We wanted to find that line. How much can we compress these LLMs before they start behaving in a manner that is less useful?,” he said.

The rapid pace of LLM development raises new questions even as researchers answer existing ones. And with growing emphasis on this technology among the AI/ML community and at top conferences, understanding how LLMs work is the key to realizing their potential.

“By performing large-scale empirical studies, we observed certain compression algorithms improve the performance of LLMs while others harm the performance,” Diffenderfer said. “These results are valuable for producing efficient, trustworthy models in the future or designing improved architectures that are intrinsically more efficient and trustworthy.”

More valuable models

Livermore’s LLM research extends beyond these papers and reveals important insights into the high-stakes arena of AI safety, which is the focus of the October 2023 White House Executive Order. The Laboratory Directed Research and Development program funds projects that tackle different aspects of safety, and the Lab’s experts continually explore ways to maximize AI/ML benefits while minimizing risks. (Visit the Data Science Institute’s website for a list of high-profile publications on these topics.)

“Any major technological breakthrough results in both positive and negative impacts. In the Department of Energy and national security context, AI technologies come with the responsibility to be safe and secure,” Kailkhura said. “I have been working on this problem for a while now, and I am pretty confident that we will improve powerful AI models and solve key scientific challenges with them. We need to be proactive and move quickly.”

Accelerating material characterization: Machine learning meets X-ray absorption spectroscopy

Lawrence Livermore National Laboratory (LLNL) scientists have developed a new approach that can rapidly predict the structure and chemical composition of heterogeneous materials.

In a new study in ACS Chemistry of Materials, LLNL scientists Wonseok Jeong and Tuan Anh Pham developed a new approach that combines machine learning with X-ray absorption spectroscopy (XANES) to elucidate the chemical speciation of amorphous carbon nitrides. The research offers profound new insights into the local atomic structure of the systems, and in a broader context, represents a critical step in establishing an automated framework for rapid characterization of heterogeneous materials with intricate structures.

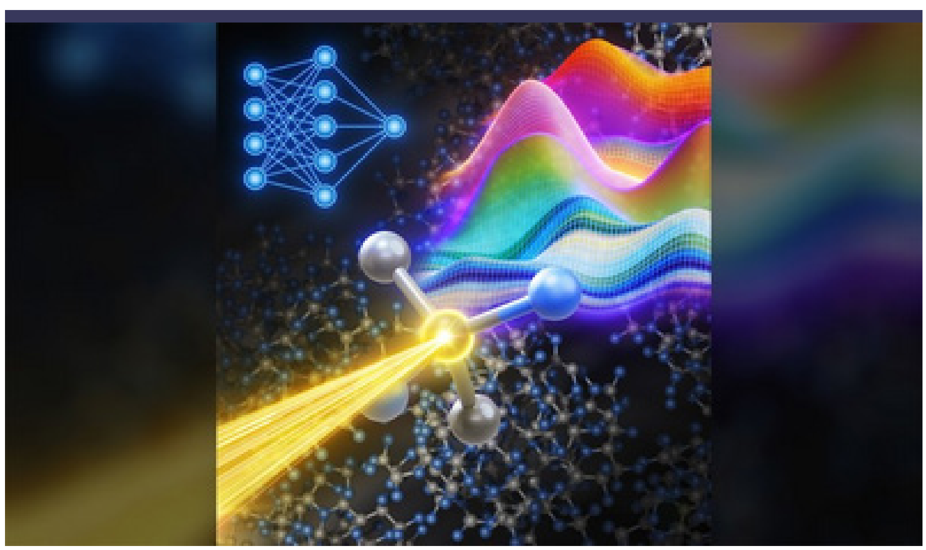
Principal Investigator: Tuan Anh Pham

LDRD Project: 22-ERD-014

Automated Characterization of Heterogeneous Materials: A Case Study Using X-Ray Absorption Spectroscopy of Detonation Products

Unraveling the atomic structure of heterogeneous materials, such as carbonaceous residues produced from the detonation of high explosives, has posed a significant challenge to materials scientists. The process is often labor-intensive, and in many cases, involves the use of empirical parameters.

To address this outstanding challenge, the team's integrated approach begins with the development of machine-learning potentials capable of efficiently exploring the vast configuration space of amorphous carbon nitrides as a representative system. This neural-network-based model enables the identification of representative local structures within the material, providing insights into how these structures evolve with chemical compositions and density.



Artwork illustrating a new study combining atomistic simulations, machine learning potential, and data-driven methods to study the chemical speciation of amorphous carbon nitride using X-ray absorption near-edge structure (XANES) spectra. (Illustration concept: Wonseok Jeong and Tuan Anh Pham/LLNL; Illustration: Ella Maru Studios)

By coupling these machine-learning potentials with high-fidelity atomistic simulations, the researchers establish correlations between local atomic structures and spectroscopic signatures. This correlation serves as the basis for interpreting experimental XANES data, allowing for the extraction of crucial chemical information from complex spectra.

"In our study, we aimed to tackle the longstanding challenge of characterizing detonation products and disordered materials in general by integrating computational methods with experimental techniques," said Jeong, the first author of the paper.

"Our approach not only enhances our understanding of these materials but also lays the groundwork for similar studies across different material systems and characterization methods. For example, the approach can be readily employed to predict elemental speciation for a broad range of carbonaceous residues and provide inputs for improving detonation models," said Pham, the principal investigator of the project.

The study's findings represent a significant advancement in the field of materials science, offering a robust framework for elucidating the atomic speciation of disordered systems. Moreover, the versatility of the approach means it can be readily adapted to investigate other materials classes and experimental characterization probes, paving the way for real-time interpretation of spectroscopic measurements.

Germanium isotope really does have an 11-day half-life

Searching for the elusive neutrino takes on many forms. Detectors consisting of many tons of gallium are used in several experiments because neutrino interactions can occur on the stable gallium-71 (71Ga) nucleus and transform it into a radioactive isotope of germanium (71Ge) with an 11-day half-life that can then be observed with traditional radiation detectors.

However, the rate of 71Ge production from these interactions has been observed to be short of expectations. This has emerged as what is referred to as "the gallium anomaly" — a significant discrepancy that occurs when electron neutrinos bombard gallium and produce the 71Ge.

This anomaly cannot be explained by current theories. As a result, it has given rise to speculation that it could be a signature that the neutrino can transform into other exotic particles, such as sterile neutrinos, which interact even less with matter than a normal neutrino; if confirmed, this would be a massive discovery.

Recently, a suggestion was made that this anomaly could instead be explained by something more mundane – a mismeasured half-life for the 71Ge nucleus. This is because the predicted rate of neutrino interactions depends on this half-life.

To test this possible explanation of the gallium anomaly, a team of scientists from Lawrence Berkeley and Lawrence Livermore national laboratories have determined the 71Ge half-life with a set of carefully performed measurements including two performed side-by-side with other long-lived radioactive isotopes with well-known half-lives. The

Principal Investigator: Nicholas Scielzo

LDRD Project: 23-SI-004

The Biggest Bang for Your Buck: Pioneering a Nuclear-Science Program Guided by Artificial Intelligence

A team of scientists from Lawrence Berkeley and Lawrence Livermore national laboratories have determined the 71Ge half-life with a set of carefully performed measurements. The research appears in the journal Physical Review C.

research appears in Physical Review C.

The team was able to pin down the 71Ge half-life to a precision about four times better than any previous measurement. The work eliminates the mismeasurement of 71Ge as an explanation for the anomaly, which thus must have a different origin — possibly in the existence of a fourth neutrino type, called a sterile neutrino.

"The new half-life obtained by our team confirmed the earlier results, but put it on much firmer footing, definitively ruling out the possible explanation that the missing neutrinos were instead due to an incorrect 71Ge half-life," said LLNL scientist and co-author Nick Scielzo. "Therefore, the gallium anomaly remains a true mystery – one that potentially still requires some kind of unexpected new neutrino behavior to understand."

It's getting hot in here: lasers deliver powerful shocking punch

Shock experiments are widely used to understand the mechanical and electronic properties of matter under extreme conditions, like planetary impacts by meteorites. However, after the shock occurs, a clear description of the post-shock thermal state and its impacts on material properties is still lacking.

Lawrence Livermore National Laboratory (LLNL) scientists used ultra-fast X-ray probes to track the thermal response of aluminum and zirconium on shock release from experiments and found the resulting temperatures were much higher than expected. The research appears in the Journal of Applied Physics.

Principal Investigator: Jon Belof

LDRD Project: 21-SI-006 and 16-ERD-037

Project DarkStar, Ultrafast Shock Kinetics of High-Z Materials with High Throughput

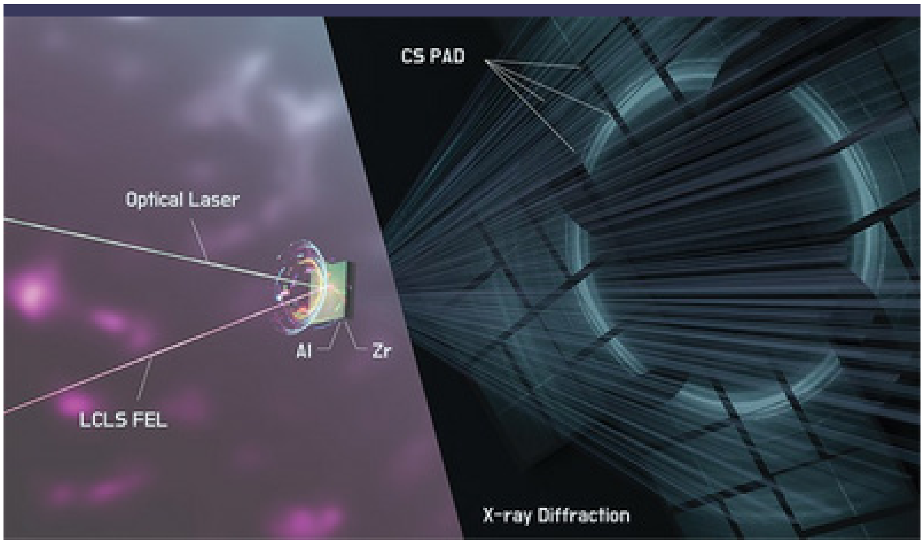
A shock wave is a large-amplitude mechanical wave across which pressure, density, particle velocity, temperature and other material properties change abruptly as the wave travels through the material. The shock compression process is thermodynamically irreversible, where a substantial portion of the energy in a shock wave goes into raising the entropy and temperature of the material.

The team used diffraction patterns from 100-femtosecond X-ray pulses to investigate the temperature evolution of laser-shocked aluminum-zirconium metal film composites at time delays ranging from 5 to 75 nanoseconds driven by a 120-picosecond short-pulse laser.

"We found significant heating of both the aluminum and zirconium after shock release, which can be attributed to heat generated by inelastic deformation," said LLNL principal investigator Harry Radousky, a co-author of the study.

As it turns out, a conventional hydrodynamic model that uses typical descriptions of aluminum and zirconium mechanical strength and elevated strength responses (which might be attributed to an unknown strain rate) did not fully account for the measured temperature increase, which suggests that other strength-related mechanisms could play an important role in thermal responses under shock wave loading/unloading cycles.

"What we found is that a significant portion of total shock energy delivered by lasers become heat due to defect-facilitated plastic work, leaving less converted to kinetic energy," said LLNL scientist Mike Armstrong, another co-author of the study. "This heating effect may be common in laser-shocked experiments but has not been well acknowledged. The high post-shock temperatures may induce phase transformation of materials during shock release."



Femtosecond X-ray diffraction of laser shocked aluminum-zirconium metals. (Image: Ji-In Jung/Stanford)

Armstrong said another potential application of the study is preserving magnetic records from planetary surfaces that have a shock history from frequent impact events.

Using xhe Matter in Extreme Conditions instrument at the Linac Coherent Light Source, the team found results showed much higher residual temperatures than expected from standard hydrodynamic release simulations, indicating there are other heat generating processes (void formation is one example) occurring during the release not usually included in these models.

Lab physicists announce significant advance in controlling instability in hydrodynamics

In a study published in the journal Physical Review Letters and noted as an Editor's Suggestion, a team of physicists at LLNL have announced a significant scientific advance in controlling Richtmyer-Meshkov instability (RMI) in hydrodynamics. The team showed that specific sequences of shockwaves can effectively manage RMI, a phenomenon commonly observed in fluid dynamics when different densities of materials interact under shockwave conditions. Understanding RMI is highly important for laser-driven inertial confinement fusion (ICF) such as is pursued at the National Ignition Facility (NIF). RMI severely degrades ICF performance, so its mitigation may be viewed as an important steppingstone toward clean energy via fusion.

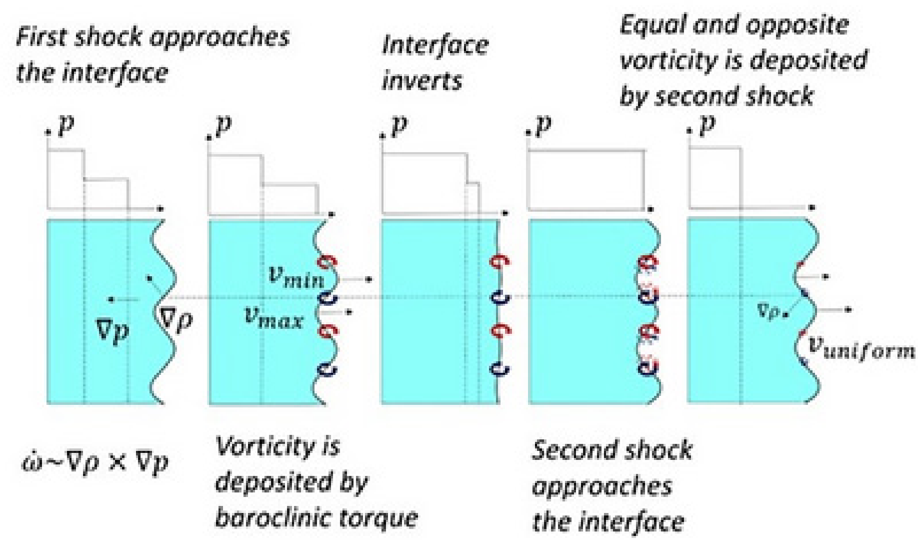
Principal Investigator: Jon Belof
LDRD Project: 21-SI-006
Project DarkStar

The study outlines two methods for generating these controlling shockwaves: a tailored drive approach and a material phase transition technique. The tailored drive method involves precise manipulation of shockwave intensity and timing, whereas the phase transition technique leverages changes in the material's state to induce the necessary shockwaves. In both scenarios, the underlying physical mechanism — discovered through extensive physics simulation work — is the same, relying upon the generation of vortices (regions of spinning or swirling material) after passage of the shockwave.

"Imagine part of a fluid that is spinning, like what happens if you pull the plug at the bottom of a bathtub. That vortex motion happening at a small scale is ultimately responsible for causing RMI and jetting when a shockwave breaks out of a material," said lead author of the study William Schill, staff scientist and deputy group leader of Material Dynamics and Kinetics in the Materials Science Division at LLNL. Schill elaborates further: "It turns out that, for very special conditions that we can create, it is possible to generate vortices that spin in the opposite direction, cancelling out the vortices generated by the shock and stabilizing the interface. In the case of a material undergoing phase transition from one state to another, the material may automatically suppress RMI, so to speak."

To put the new theory to the test, an experimental campaign was conducted with team members at the Special Technology Laboratory (MSTS) in Santa Barbara, California, to generate the needed shockwaves under impact of a high-speed projectile. Firing a bullet at over 5,000 miles per hour and slamming it into a stationary piece of iron, a strong shockwave was generated that compressed the iron to a very high pressure. On the back of the sample were intentionally placed defects that are known to cause the hydrodynamic instability to form. Over a time period of several millionths of a second, x-ray images of the instability were taken and compared with theoretical predictions; remarkably, the instability was suppressed in agreement with the new vorticity cancellation theory. Mike Armstrong, deputy group leader in the Materials Science Division and the lead scientist for the experimental campaign, said: "We were surprised and excited by the results of this experimental campaign — the data from the shots showed very clearly that the method of controlling RMI worked exactly as predicted, demonstrating the practical feasibility of this approach in real-world scenarios."

The control of Richtmyer-Meshkov instability has profound implications across multiple scientific fields, including inertial confinement fusion, astrophysics, materials science and energy research. This discovery may open new avenues for research in controlling high-velocity impacts and explosions, potentially leading to advancements in protective materials design and energy harnessing methods. The approach relied on use of advanced supercomputing resources and multiphysics simulation codes, highlighting the cutting-edge scientific capabilities provided to the U.S. by the Department of Energy laboratories.



The mechanism of how the interface instability is suppressed: double shock wave propagates (moving in a direction toward the right) through the material, depositing vorticity at the interface with a specific timing wherein the second vorticity deposition cancels the first due to the inversion of the wave profile.

Revolutionary tool speeds up GPU programs for scientific applications

Principal Investigator: Konstantinos Parasyris

LDRD Project: 23-ERD-022

Localizing and Explaining Performance Defects in Heterogeneous Applications

A Lawrence Livermore National Laboratory (LLNL)-led team has developed a method for optimizing application performance on largescale graphics processing unit (GPU) systems, providing a useful tool for developers running on GPU-based massively parallel and distributed machines.

A recent paper, which features four LLNL co-authors, describes a mechanism called Record-Replay (RR), which speeds up applications on GPUs by recording how a program runs on a GPU, and then replaying that recording to test different settings and finding the fastest way to run the program. The paper was a finalist for the Best Paper award at the 2023 International Conference for High Performance Computing, Networking, Storage and Analysis (SC23).

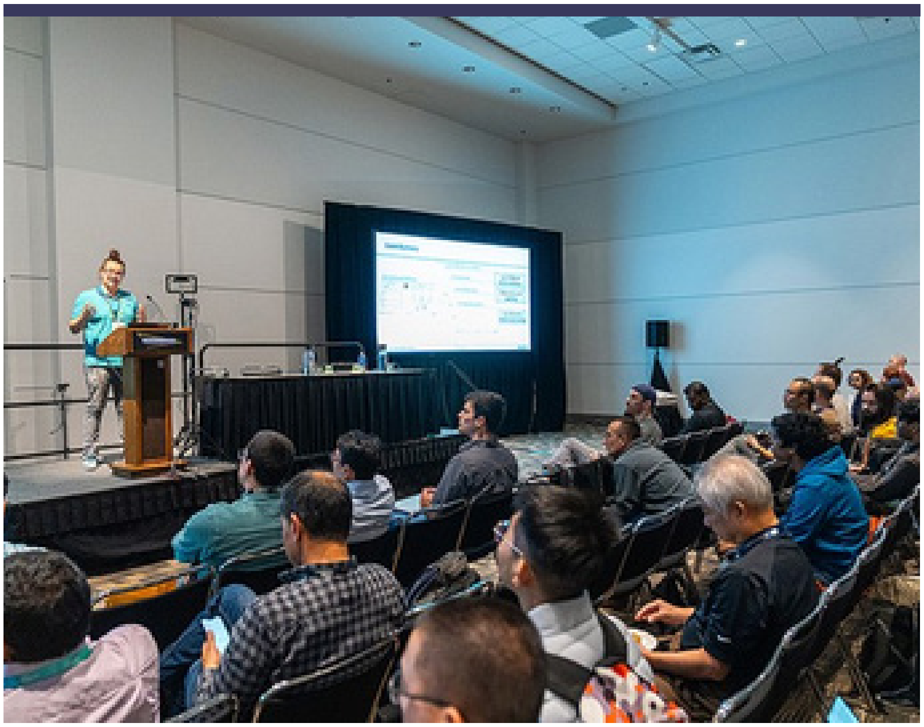
"We developed a tool that automatically picks up part of the application, moves it as an independent piece so you can start independently and then optimize it," said lead author and LLNL computer scientist Konstantinos Parasyris. "Once it is optimized, you can plug it into the original application. By doing so you can reduce the execution time of the entire application and do science faster."

In the paper, the authors describe how RR works and how it can be used to improve the performance of OpenMP GPU applications. Parasyris said the mechanism helps "autotune" large offload applications, thus overcoming a major bottleneck for speed in scientific applications.

As a case study, the authors demonstrated how RR was used to optimize performance of LULESH, a shockwave hydrodynamics code that simulates the behavior of materials under stress. By using the Record-Replay mechanism, researchers were able to optimize LULESH to run up to 50% faster on GPUs, an improvement that could make it possible to simulate much larger and more complex materials, key for many scientific and engineering applications.

"You can directly translate that as a 50% speed-up on an application," Parasyris said. "Science is driven by how fast you can do observations, and in that case, we'll be able to increase the number of observations within a day; so, the [calculation] that previously took a day to do, would only take two-thirds of the day."

By using the RR mechanism, researchers said they can test many different settings quickly and efficiently, making it possible to use Bayesian optimization — a method for finding the optimal settings for a program by



Lawrence Livermore National Laboratory computer scientist Konstantinos Parasyris presents his team's paper on the Record-Replay technique for speeding up applications on GPU-based systems at the 2023 International Conference for High Performance Computing, Networking, Storage, and Analysis (SC23). Photo courtesy of SC

testing different options and using statistics to determine which ones work best — on very large programs that would otherwise be too time-consuming to optimize.

"Every program has many parameters that you can use to optimize it, and those parameters can be combined if it's out there," said LLNL scientist and co-author Giorgis Georgakoudis said. "If you find the best way to combine them, you can significantly reduce the execution time of the application, so that's our goal."

Researchers said they plan to continue the work by investigating more use-cases facilitated by RR, such as tuning the compiler optimization pipeline, automatic benchmark generation and automated testing and debugging.

In addition to the Best Paper finalist, Parasyris and Georgakoudis also co-authored a paper presented at SC23 by LLNL intern Zane Fink on HPAC-Offload, a programming model allowing portable approximate computing (AC) to accelerate HPC applications on GPUs. The technique involves identifying and selectively approximating parts of the application that have low significance, resulting in significant performance improvements while minimizing quality loss.

The authors demonstrated the effectiveness of HPAC-Offload on several HPC benchmarks, conducting a comprehensive performance analysis of the tool across GPU-accelerated HPC applications. They found that AC techniques can significantly accelerate HPC applications (1.64x LULESH on AMD, 1.57x on NVIDIA GPUs) with minimal quality loss (0.1%). The team also provided insights into the interplay between approximate computing and GPU-based parallelism, which can guide the future development of AC algorithms and systems for these architectures. That paper also includes LLNL computer scientist Harshitha Menon as a co-author.

Unlocking gas phase uranium oxidation is key to nuclear debris modeling

Principal Investigator: Kimberly Knight

LDRD Project: 20-SI-006

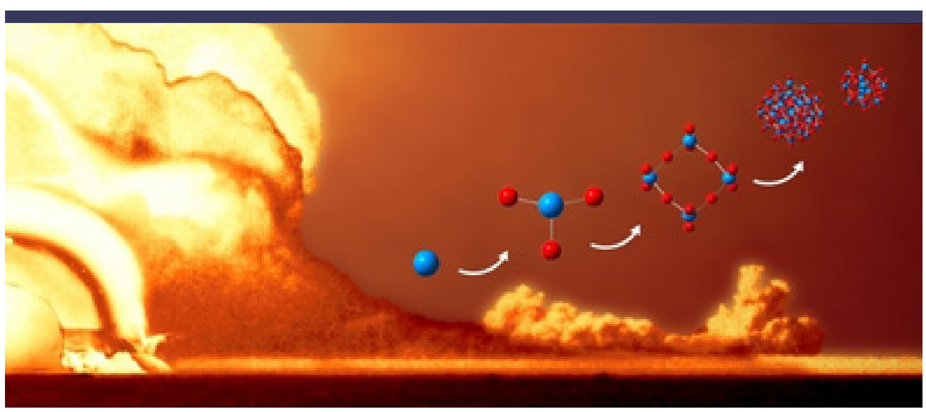
Identifying the Influence of Environmental Effects on Post-Detonation Chemistry and Debris Formation

In the quest to understand how nuclear debris forms, a team of scientists at Lawrence Livermore National Laboratory (LLNL) has developed an approach to studying the oxidation mechanism of gas phase uranium in extreme environments.

In research recently published in Scientific Reports, the team outlined their work, which combined experimental data from a plasma flow reactor — a unique experimental platform built at LLNL — with advanced computational techniques to shed light on the intricate mechanics of gas phase uranium oxidation at atmospheric pressure.

By employing a Monte Carlo genetic algorithm, a hybrid model that uses random sampling and natural selection, researchers optimized a reaction mechanism based on optical emission spectra measurements from the plasma flow reactor, explained Mikhail Finko, lead researcher on the project. Using this method, reaction rates of gaseous uranium oxidation were then backed out from experimental data instead of being calculated from first principles.

"The methodology we employed not only identifies dominant reaction



To better understand how nuclear debris forms, Lawrence Livermore National Laboratory scientists have refined the optimization of a uranium oxide reaction mechanism using plasma flow reactor measurements and advanced computational methods. (Image courtesy of Mikhail Finko/LLNL) pathways and rates but also paves the way towards producing a comprehensive, experimentally validated reaction mechanism, a crucial element for modeling nuclear debris formation," Finko said.

The algorithm LLNL researchers used identified four dominant reaction pathways for forming diatomic uranium oxides and determined the corresponding reaction rates. Furthermore, due to the presence of water in the system, the optimization identified the hydroxyl (OH) radical, a highly reactive chemical species composed of oxygen and hydrogen, as a dominant molecule for producing uranium oxides.

In part due to the development of convenient experimental systems for studying gas phase uranium chemistry, the subject has seen increased interest in recent years. While advances in qualitative understanding of gaseous uranium oxidation mechanics have been made, obtaining validated quantitative reaction rates has remained a challenge, Finko said. The results of this research are directly relevant for the field of material chemistry in extreme environments, as existing reaction mechanisms are not yet well validated.

LLNL researchers develop framework for databasing properties of crystal defects

Point defects (e.g. missing, extra or swapped atoms) in crystalline materials often determine the actual electronic and optical response of a given material. For example, controlled substitutions in semiconductors like silicon are the backbone of modern technology. Despite their importance, point defects are notoriously difficult to simulate and characterize, particularly across wide regions of the periodic table.

Researchers at Lawrence Livermore National Laboratory (LLNL) have now created software as part of its open-source software distribution that can efficiently and effectively automate and analyze these types of calculations.

The authors demonstrated the fully automated approach on several technologically important materials. including gallium nitride (the basis of all modern solid-state lighting), gallium oxide (an emerging ultrawideband gap semiconductor) and strontium titanate (a widely studied common mineral), with the work recently published in the Journal of Applied Physics and selected as an Editor's Pick as part of a special issue on "Defects in Semiconductors."

"This work has enabled us to look more systematically at different types of defects in materials that exhibit the behavior we have been looking for," said Lars Voss, a co-author of the work.

"We have been doing these types of calculations by hand for years, but modern advances in high-throughput computing and database software have made this a more practical and flexible approach," said LLNL scientist Joel Varley, also a contributing author on the paper.

The study and open-source software developed as part of the project has attracted interest from a number of international research teams and industry, the researchers said.

Principal Investigator: Lars Voss

LDRD Project: 22-SI-003

Ultrawide Bandgap Laser Addressable Photoconductors

"Now that we have developed a framework to streamline this approach with modern databasing practices, this opens up a straightforward path to curate data for machine-learning approaches to be systematically applied to point-defect properties by the community," said Jimmy Shen, lead author on the paper.

Left to right: LLNL researchers Jimmy Shen, Lars Voss and Joel Varley have software that can efficiently and effectively automate and analyze point defects in materials. (Photo: Blaise Douros/LLNL)

Scientific Leadership and Service

LDRD projects are distinguished by their mission-driven creativity. LDRD-funded research often launches stellar careers, initiates strategic collaborations, produces game-changing technical capabilities, and even lays the foundation for entirely new fields of science. It is no surprise that every year, LDRD principal investigators from LLNL are recognized for the groundbreaking results of a project or long-term contributions to their fields. The following examples highlight recognition received during fiscal year 2024, attesting to the exceptional talents of these researchers and underscoring the vitality of Livermore's LDRD Program.

NEW FELLOW

LLNL's Raspberry Simpson, selected as a National Academy of Sciences (NAS) Kavli Fellow, presented a poster on her postdoctoral fellowship at the academy's annual Kavli Frontiers of Science symposium. (Photo courtesy of Raspberry Simpson)

LLNL's Raspberry Simpson named Kavli Fellow

Raspberry Simpson, a Lawrence Fellow in Lawrence Livermore National Laboratory's (LLNL) National Ignition Facility and Photon Science (NIF&PS) Directorate, has been named a National Academy of Sciences (NAS) Kavli Fellow.

As a new Kavli fellow, Simpson participated recently in the annual NAS Kavli Frontiers of Science symposium in Irvine, California. NAS invited outstanding young scientists to discuss advances and opportunities in a wide variety of disciplines, including astrophysics, space science, space technology and xenobots — synthetic lifeforms made from components of living cells designed to perform robotic functions.

"It was definitely an honor to be invited to attend this meeting and to be able to meet other early-career scientists in other fields and learn about the NAS, which has the mission to inform the government on a wide array of scientific topics," Simpson said. "I was able to make important connections with scientists outside of my field, such as individuals from Lawrence Berkeley National Laboratory that work in astrophysics and people from NASA Goddard."

The Goddard Space Flight Center is the National Aeronautics and Space Administration's premiere space flight complex in Greenbelt, Maryland.

"I'm happy to be included in the NAS and Kavli communities and hope to be able to contribute in the future on their reports on high-energy-density (HED) science, high-brightness sources or fusion energy," she said.

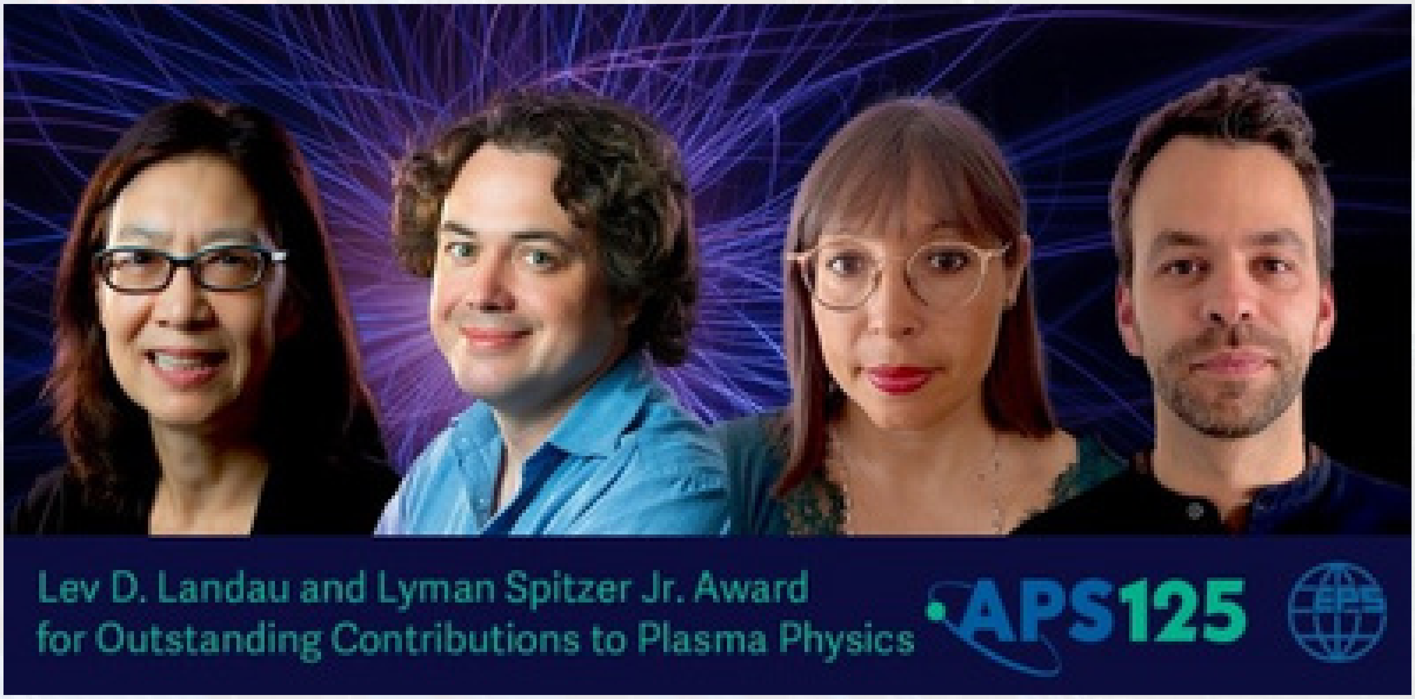
Simpson presented a poster on her postdoctoral fellowship titled "Investigation of Boosted Proton Energies in the Multi-ps Regime for Applications to Proton Fast Ignition."

"It was a nice experience to be able to practice my own scientific communication and explain my work to individuals who are not necessarily in my field," she said.

Simpson joined LLNL in 2022. She works on developing new experimental and machine-learning tools to optimize laser-driven secondary particle sources. Her work aims to address the need for next-generation diagnostics, machine-learning methods and analysis tools to be able to perform laser experiments at faster rates.

Simpson received her Ph.D. in nuclear engineering with a focus on plasma physics from the Massachusetts Institute of Technology. She completed most of her Ph.D. research at LLNL under the direction of physicist Tammy Ma, focusing on the investigation of laser-driven particle acceleration for the development of tunable ion sources for applications in HED science.

Two LLNL physicists honored for international collaboration



Left to right: Hye-Sook Park (LLNL), George Swadling (LLNL), Anna Grassi and Frederico Fiuza. (Graphic: Amanda Levasseur/LLNL)

Lawrence Livermore National Laboratory (LLNL) physicists Hye-Sook Park and George Swadling, along with Anna Grassi of France's Sorbonne University and former Lawrence Fellow Frederico Fiuza of Portugal's Técnico Lisboa, received the 2024 Lev D. Landau and Lyman Spitzer Jr. Award for Outstanding Contributions to Plasma Physics. The award is jointly sponsored by the Plasma Physics Divisions of the American Physical Society and the European Physical Society.

The team was cited for "critical advancement in the understanding of the particle acceleration physics in astrophysically relevant shocks through theoretical analysis and experiments at the National Ignition Facility."

"It is an honor to receive this award," Park said. "We have been studying collision-less shocks in the laboratory using high-power lasers such as NIF and Omega by creating similar conditions in dimensionless units. We were particularly interested in how cosmic ray particles are accelerated to very high energy." Many theories exist, but observing the exact mechanisms is difficult.

"The physics of collision-less shocks is fascinating," Swadling said. "They are common in astrophysics, forming, for example, at the interface between expanding supernova explosions and the interstellar medium. Only with the laser power and energy available at NIF are we able to design experiments at the spatial and temporal scales required to study their formation in the laboratory."

This work showed that the electrons in the high-velocity plasma gain enough energy through the interplay of self-generated magnetic fields and the shock front, and these electrons are injected into another acceleration mechanism called a first-order Fermi process. The novel diagnostics on NIF measuring particle acceleration and the plasma conditions with novel simulations enabled these findings.

Two LLNL researchers named to Optica's 2024 class of senior members

LLNL's Brent Stuart and Paul Armstrong have been named Optica senior members.

Lawrence Livermore National Laboratory (LLNL) researchers Paul Armstrong and Brent Stuart have been named senior members of Optica. The professional society's senior membership status recognizes members with more than 10 years of professional experience in optics or an optics-related field.

The 2024 class joins a distinguished group of scientists, engineers, entrepreneurs and innovators who have demonstrated exemplary professional accomplishments in optics and photonics.

Paul Armstrong

Armstrong, an engineer in the National Ignition Facility and Photon Science Directorate, manages an effects laboratory in the Department of Defense Technologies program and investigates challenging problems in material science and laser-matter interaction.

"I feel fortunate to have spent my entire career at LLNL tackling difficult problems of national importance, supported by one of the best workforces around," he said. "When you combine that with the opportunities afforded by Optica, amazing things happen. I am honored to have been selected as a senior member of such a respected professional society."

Armstrong earned his bachelor's degree in Laser Optical Engineering Technology from the Oregon Institute of Technology and immediately joined LLNL. He began his career performing research in femtosecond lasers and their applications, including hardware-centric evolutionary algorithms and advanced control systems. He subsequently shifted focus to developing early concepts in inertial fusion energy drivers and other solid-state laser front-ends, such as the L3 HAPLS (High-Repetition-Rate Advanced Petawatt Laser System) now

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installed at ELI-Beamlines in the Czech Republic. Over his 30 years of work in photonics-related research, he has developed several novel instruments and processes, garnering multiple patents and three R&D100 awards. His current research concentrates on infrared imaging, spectroscopy and thermography.

Brent Stuart

Stuart, a staff scientist in the Physical and Life Sciences Directorate, is the operations manager for the Jupiter Laser Facility (JLF). He oversees all aspects of laser development and innovation at JLF. Recently, he led a large facility modernization effort for the facility, which resulted in multi-million-dollar investments by LLNL and the DOE Office of Science to redesign and rebuild the laser beamlines, power conditioning systems and diagnostics. The laser reopened for user experiments in 2023.

"I'm honored by this recognition, and thankful for all the exciting opportunities and amazing colleagues here at LLNL that made this award possible," Stuart said.

He earned his bachelor's degree in physics from Caltech and his Ph.D. in engineering/applied science from the University of California, Davis. After demonstrating a new ultraviolet laser based on the sulfur monoxide molecule for his thesis work, Stuart joined LLNL to work on the Nova petawatt laser, where he built up the front-end of the system and performed seminal investigations into the mechanisms of sub-picosecond laser ablation and materials processing applications.

Stuart also has delivered femtosecond machining systems to the Y-12 Plant and LLNL's High Explosives Applications Facility; the trigger laser for the Dynamic Transmission Electron Microscope; and novel active remote-sensing systems. His leadership in laser design and operations led to many applications in particle acceleration, high-field laser-matter interactions, materials characterization, remote sensing and materials processing. Stuart has served on many major Optica conference program committees such as CLEO, Photonics West and Frontiers in Optics.

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LLNL's Gauthier Deblonde selected as 'Rising Star'

LLNL staff scientist Gauthier Deblonde has been selected as a "Rising Star" by the American Chemical Society. (Image: Eric Smith/ LLNL; Photo: Garry Mcleod/LLNL)

Lawrence Livermore National Laboratory (LLNL) staff scientist Gauthier Deblonde has been named a 2024 "Rising Star" by the American Chemical Society for his work in environmental science.

Deblonde's research as well as this year's cohort of winners will be featured in a special issue of the American Chemical Society journal ACS Environmental Au. Deblonde's research also has been selected for the front cover of the journal's current issue.

As a staff scientist in LLNL's Nuclear and Chemical Sciences Division in the Physical and Life Sciences Directorate, Deblonde's work focuses on developing new techniques to decipher the chemistry of radioactive elements.

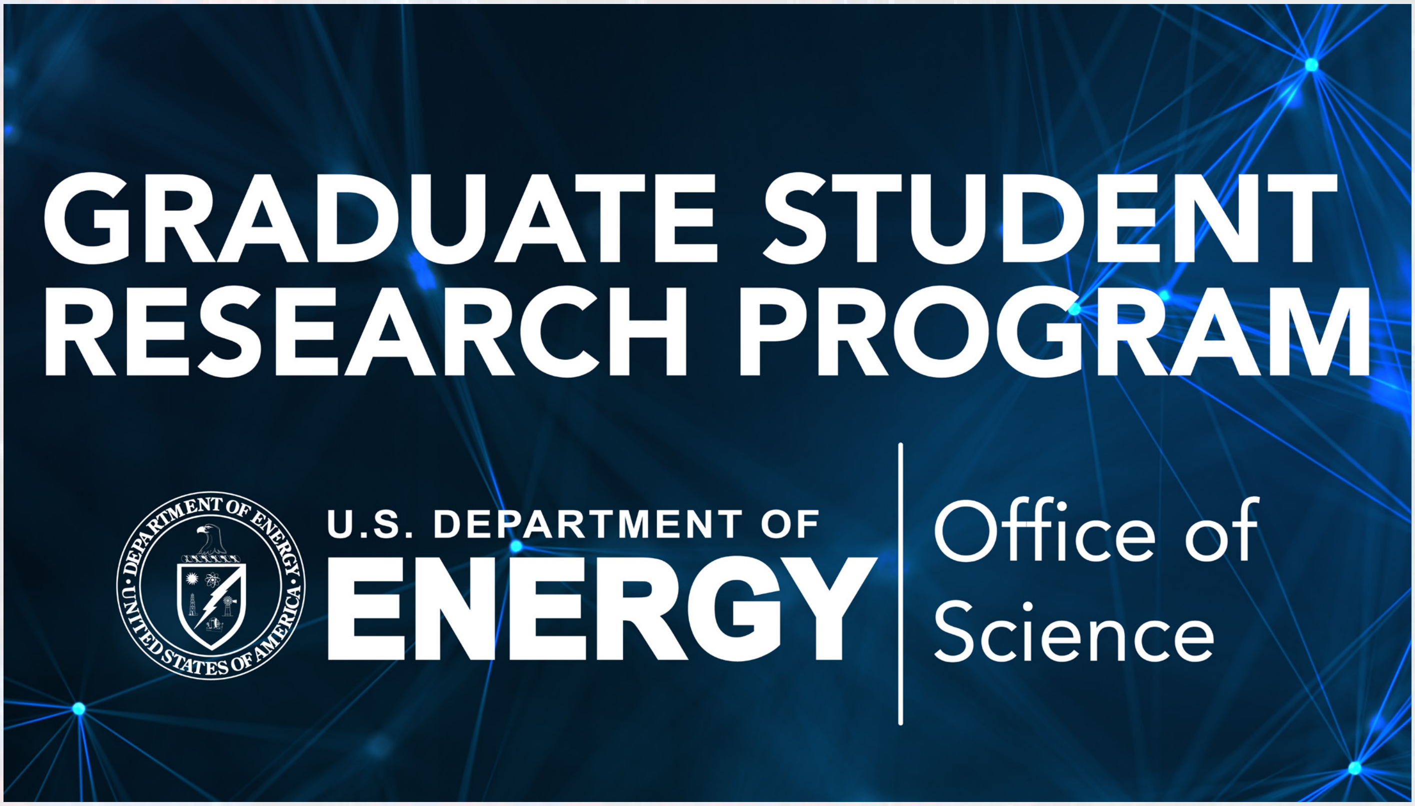
Deblonde has always been fascinated by "difficult-to-study" materials. So, he naturally turned to nuclear sciences, and particularly the chemistry of heavy elements and "actinides" (a family of 15 radioactive elements, which includes uranium and plutonium).

Most of these elements only exist in trace amounts in nature or need to be produced in nuclear reactors and, as a result, we know very little about their chemical properties – relative to other non-radioactive materials. Deblonde's research focuses on developing new strategies to probe the chemistry of these rare, toxic and elusive chemical elements.

"Most people fear radioactive materials, but a lot of this is irrational and not based on facts," he said. "That's why it is important to study such materials — from fundamental research to applied sciences — so that we better understand their interactions with the environment, prevent potential hazards and still take full advantage of their truly unique properties for national security and civilian applications."

Current studies in his lab focus on the interactions between metal ions and chelators (natural small molecules, polyoxometalates, synthetic ligands or macromolecules, like proteins). Such studies have broad implications, ranging from separation technologies and medical applications to nuclear sciences, strategic metal mining and the environmental behavior of heavy metals.

Three selected as Graduate Student Research program recipients



Ricardo Monge Neria from Case Western Reserve University, Andrew Marino from the Colorado School of Mines and Anthony Stewart from the University of Washington will arrive at the Lab this summer to start their fellowships.

Three graduate students have earned Department of Energy (DOE) Office of Science Graduate Student Research (SCGSR) Program awards to perform their doctoral dissertation research at Lawrence Livermore National Laboratory (LLNL). The prestigious award helps cover living expenses and travel for 60 students from universities across the nation. Their proposed research projects address scientific challenges central to Office of Science mission areas from nuclear physics to environmental systems and advanced manufacturing.

"The Graduate Student Research program is a unique opportunity for graduate students to complete their Ph.D. training with teams of world-class experts aiming to answer some of the most challenging problems in fundamental science," said Harriet Kung, acting director of the DOE Office of Science. "Gaining access to cutting-edge tools for scientific discovery at DOE national laboratories will be instrumental in preparing the next generation of scientific leaders."

Andrew Marino from the Colorado School of Mines, Ricardo Monge Neria from Case Western Reserve University and Anthony Stewart from the University of Washington will arrive at the Lab this summer to start their fellowships.

Through world-class training and access to state-of-the-art facilities and resources at DOE national laboratories, SCGSR prepares graduate students to enter jobs of critical importance to the DOE mission and secures the national position at the forefront of discovery and innovation.

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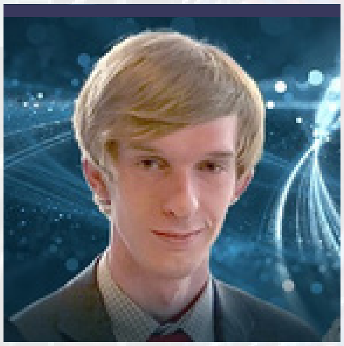


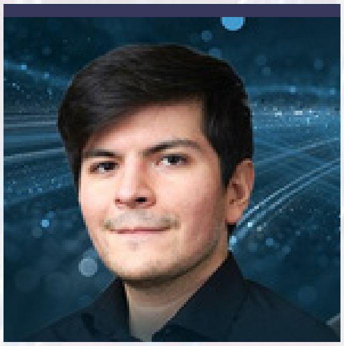
ANDREW MARINO

Under the direction of staff scientist Stephan Friedrich, Marino will continue to contribute to a sterile neutrino project with superconducting radiation detectors (nicknamed the "BeEST"), that he started working on while taking classes at Colorado School of Mines.

"I'm super excited to have received the SCGSR award and to have the opportunity to work here to further my thesis research with Stephan," Marino said. "I've been mostly working with the data taken with our detectors by someone else and am really looking forward to taking some data myself."

In school, Marino worked with Superconducting Tunnel Junction (STJ) radiation detectors to measure nuclear recoils. While at LLNL, he will work on the method of STJ detector calibration. In the past, the team has used a laser to compare the energy of laser photons (easily measured) to that of the nuclear recoils (much harder).

"However, nobody has confirmed yet that there's no weird offset associated with low-energy events [missing some photons, for instance] or the difference between photons and charged particles [i.e. nuclei]," Marino said. "I'm hoping that I'll get some great data from STJs and confirmation that our calibration methodology is working accurately."

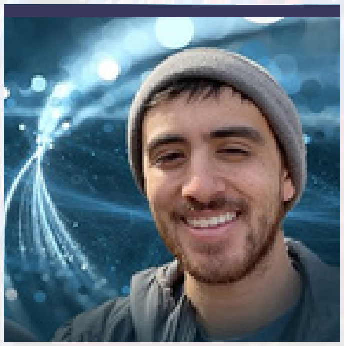


RICARDO MONGE NERIA

As a physics student specifically studying techniques to optimize chemical separations, Monge Neria will work under the direction of staff scientist Dan Park on rare-earth element (REE) research. He is an experimental biophysics Ph.D. candidate on paper, but his work has mostly focused on studying chemical separations through the lens of single-molecule fluorescence microscopy. He studies the materials science aspect of liquid chromatography-based chemical separations, studying different porous and functionalized materials for difficult separations like rare earths and chiral chemicals.

Monge Neria will work with Park's team to study protein-based approaches for the separation of crucial rare-earth metals, including measurements for an application to remove metals in waste streams.

"This is a great chance to simultaneously broaden my research skills into more biological and physical chemistry techniques, as well as expand upon my thesis work," Monge Neria said. "In my mind, I like to view this opportunity as a 'mini post-doc' experience where I'll get to work more in-depth in a related research topic. And I hope to make new connections with other researchers in the field, as well as experience the unique national laboratory environment as I head into the next steps of my career."



ANTHONY STEWART

Forest ecology and soil sciences Ph.D. candidate Anthony Stewart will work under the direction of staff scientist Katerina Georgiou on soil-carbon science and persistence. Soil organic matter stores more carbon than both the atmosphere and vegetation combined, and soils in the Pacific Northwest — where Stewart conducts fieldwork — are particularly rich in carbon, in part due to the presence of forested wetlands. Importantly, this carbon also can be hundreds to thousands of years old, but it is still uncertain in what forms this soil carbon is stored and how stable it is in hydrologic gradients in these landscapes. Stewart's field of study is soil science; more specifically, soil carbon and how it persists in the soil and is distributed across landscapes.

"I'm grateful for the opportunity to work at such a prestigious institution with a great mentor and collaborators toward addressing key soil science challenges," Stewart said. "I'm hoping to directly assess how long soil carbon persists in the soil samples I collected. Additionally, I'm planning to measure geochemical properties to explore some of the mechanisms of carbon stabilization."

"We are really excited that Anthony was awarded this fellowship and will join us at the Lab," Georgiou said. "His SCGSR project will focus on the controls of soil-carbon science and persistence across a wetland-upland gradient in the Pacific Northwest. It is an ambitious project that will leverage key expertise and facilities at the Lab and will also complement our research program in the Nuclear and Chemical Science division."

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Félicie Albert elected vice chair of APS Division of Plasma Physics

Lawrence Livermore National Laboratory (LLNL) scientist and director of the Jupiter Laser Facility Félicie Albert has been elected to serve as vice chair of the American Physical Society (APS) Division of Plasma Physics (DDP) Executive Committee.

Established in 1959, the objective of DPP is the advancement and dissemination of the knowledge, understanding, and applications of plasmas — assemblages of charged particles of natural and laboratory origin.

In this four-year leadership commitment, Albert will serve as chair of the APS-DPP fellowship committee in the first year and then chair the program committee for the APS-DPP annual meeting in the second. In her third year of service, Albert will chair the division, where she will lead the APS-DPP executive committee in running the division, proposing new initiatives and working with APS to ensure a vibrant and thriving plasma physics community. In her fourth year, she will serve as past chair of the division.

Albert first became a member of the APS and attended the meeting of the APS-DPP as an LLNL postdoctoral researcher in 2009.

"There has never been a better time to be part of DPP," said Albert. "Scientifically, we've seen so many breakthroughs in our field and are seeing the prospects of a clean energy source provided by fusion, both from magnetic and inertial confinement, become a reality. And plasmas are so much more. They have unparalleled breadth in temperature, density, and pressures, beat particle acceleration energy-records, help us understand space and planets, devise new means of propulsion, and have the potential to revolutionize medical and industrial applications."

LLNL's Kathryn Mohror honored with prestigious technical computing award

The Association for Computing Machinery's (ACM) Special Interest Group on High Performance Computing (SIGHPC) on Sept. 3 announced it has awarded Lawrence Livermore National Laboratory's (LLNL) Kathryn Mohror with its prestigious Emerging Woman Leader in Technical Computing (EWLTC) Award.

Mohror, a Distinguished Member of Technical Staff at LLNL and deputy director of the Laboratory Directed Research and Development program, is a leading HPC researcher with a focus on input/output (I/O) and programming models and tools designed for exascale computing. The award recognizes her remarkable achievements in high-performance computing (HPC) and her dedication to advancing the HPC community through her leadership, service and mentorship, according to SIGHPC.

"I am truly honored and excited to receive the Emerging Woman Leader in Technical Computing Award from SIGHPC," Mohror said. "This recognition by my peers and the broader HPC community is incredibly meaningful to me. The award reflects the importance of collaboration, mentorship and innovation in driving our field forward. I am deeply grateful to be part of a community that values not just technical excellence, but also service, leadership and the positive impact we can have together. I am inspired to continue pushing the boundaries of what's possible in HPC and to support the next generation of leaders in our field."

A computer scientist in the Parallel Systems Group within the Center for Applied Scientific Computing (CASC) at LLNL, Mohror is widely recognized for her work on HPC input/output (I/O) performance and parallel programming. Her research focuses on developing scalable solutions for extreme-scale computing systems, enhancing their performance, reliability and usability.

"We are incredibly proud of Kathryn and excited that she has received this well-deserved recognition," said CASC Director Jeffrey Hittinger. "This award is a testament to her exceptional technical expertise, innovative research, and commitment to advancing the field of high performance computing. Kathryn's work on scalable I/O systems and checkpointing libraries has greatly enhanced our ability to leverage HPC resources for critical national security missions and scientific discoveries. Beyond her technical achievements, Kathryn has been a remarkable leader and mentor both within the Lab and the broader HPC community. Her dedication to excellence, collaboration and service has had a profound impact, and we are fortunate to have her as a member of CASC."

Mohror earned her Ph.D. in computer science in 2010, her master's degree in computer science in 2004, and her bachelor's degree in chemistry in 1999, all from Portland State University. Her innovative research has earned her several honors, including the 2022 Oppenheimer Science and Energy Leadership Program Fellowship and the 2019 DOE Early Career Research Award.

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LLNL's Gamblin named to *HPCwire's* 'People to Watch' list for 2024

The high performance computing (HPC) publication HPCwire has selected Lawrence Livermore National Laboratory computer scientist Todd Gamblin as one of its "People to Watch" in HPC for 2024. The program recognized 12 HPC professionals who "play leading roles in driving innovation within their particular fields, making significant contributions to society as a whole." Graphic courtesy of HPCwire.

The high performance computing (HPC) publication HPCwire has selected Lawrence Livermore National Laboratory computer scientist Todd Gamblin as one of its "People to Watch" in HPC for 2024.

A distinguished member of technical staff in Livermore Computing, Gamblin is best known in the HPC community for creating Spack, a popular open source HPC package management tool that won an R&D 100 Award in 2019. Spack has grown to involve more than 1,300 contributors from more than 300 organizations and was the official deployment tool for the Department of Energy's Exascale Computing Project. Spack has also become the package manager of choice for supercomputers around the world.

In addition to leading the Spack project, Gamblin is a co-founder of the High Performance Software Foundation (HPSF), a Linux Foundation project umbrella currently in the formation stage. The foundation is expected to launch in May, and seeks to build, promote and advance a portable software stack for HPC by supporting and encouraging adoption of key HPC open source software projects.

"I am honored and humbled to be recognized by HPCwire as one of their People to Watch for 2024," Gamblin said. "This honor is a testament to the collective efforts of myself and my team, collaborators on HPSF, Livermore Computing and the entire Spack community. I am proud to be featured among the luminaries on this list and acknowledged alongside them as champions for innovation in the field of HPC."

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Inaugural National Lab Research SLAM showcases early-career researchers

The 2023 National Lab Research SLAM winners pose with Jean-luc Doumont, the evening's emcee. Pictured from left: Theresa Kucinski, Sean Noble, Jean-luc Doumont, Brandon Zimmerman, an LDRD participant, and Janet Meier. Photo by Blaise Douros/LLNL.

Gathered in the Congressional Auditorium on Wednesday, Nov. 15, 2023, 17 early-career researchers used three minutes and a single slide to present their pioneering research during the inaugural National Lab Research SLAM. Representing each of the 17 Department of Energy (DOE) national laboratories, finalists presented in four research categories: Energy Security, National Security, Environmental Resilience and Scientific Discovery. Sponsored by the House Science and National Labs Caucus and the Senate National Labs Caucus, the first-of-its-kind event heightened competition and collaboration while raising visibility of the national laboratory system and federal research priorities. The winners were: Scientific Discovery: Theresa Kucinski, Los Alamos National Laboratory; National Security: Brandon Zimmerman, Lawrence Livermore National Laboratory (LLNL); Energy Security: Janet Meier, Oak Ridge National Laboratory; Environmental Resilience: Sean Noble, Savannah River National Laboratory. LLNL's Brandon Zimmerman, winner of the National Security research category, also took home the People's Choice Award.

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