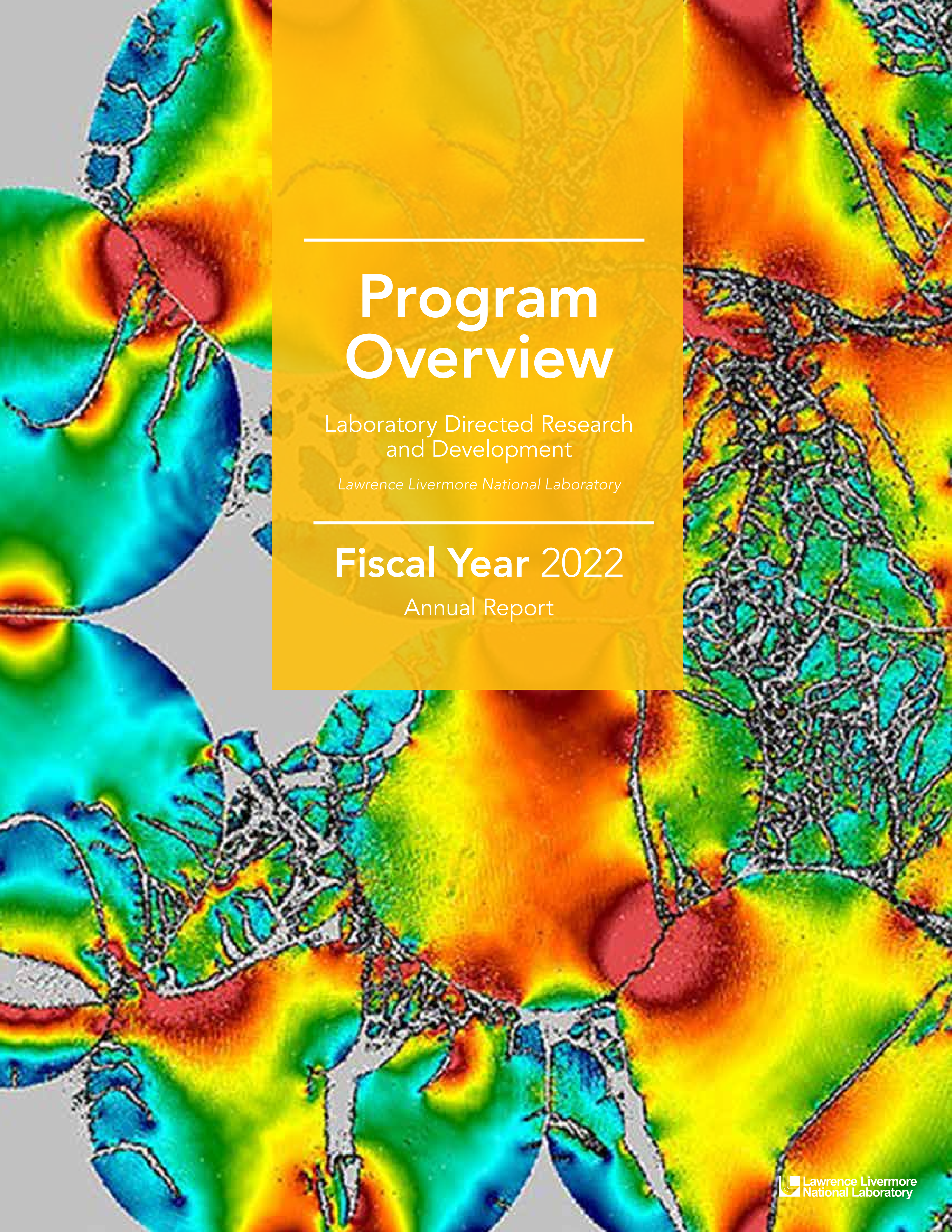

Program Overview

Laboratory Directed Research and Development

Lawrence Livermore National Laboratory

Fiscal Year 2022

Annual Report

Lawrence Livermore National Laboratory

Annual Program Overview

Director's Statement

Over the last three decades, the Laboratory Directed Research and Development (LDRD) Program has funded Lawrence Livermore National Laboratory (LLNL) research to expand the frontiers of knowledge and anticipate emerging national security challenges. In this annual report, we summarize how LLNL uses targeted investments to develop cutting-edge capabilities, advance our knowledge in strategic science and technology domains, develop our world-class workforce, and foster innovation in key programmatic areas.

LDRD investments foster mission agility through multidisciplinary research, bringing together diverse teams and collaborators to explore higher-risk innovative approaches and concepts to fulfill our mission goals. In 2022, LLNL introduced Mission Focus Areas (MFAs), program areas addressing key national and global challenges for which the laboratory's science, technology, and engineering help deliver innovative solutions. LDRD is critical in driving our science expertise, technology capacities, and renewing our position as the "big ideas" laboratory to advance our four inaugural mission focus areas: Stockpile and Enterprise Transformation, Bio-Resilience, Climate Impacts and Resilience, and Integrated Deterrence and Technology Competition. Our investments will enable agile responses to emerging national security challenges.

In addition, LDRD investments bring together diverse teams and collaborators to push the frontiers of science, technology, and engineering to ensure the technical vitality of the Laboratory. For example, investigators are using the Lab's powerful computers along with state-of-the-art experimental facilities to achieve new understanding across broad disciplines including high energy density science, advanced computing and data science, materials and manufacturing, bioscience and bioengineering, and earth and atmospheric science. As you browse this report, you will learn about cover-page publications, patents, and science awards that resulted from LDRD investments. Finally, our LDRD program cultivates the creativity of the Lab's most important resource—our workforce. LDRD-sponsored research enables outreach to tomorrow's innovators, as we mentor students, hire postdoctoral researchers, and develop the leadership capabilities of early career staff. The mentorship aspect is a hallmark of our program. A multidisciplinary group of senior scientists and advisors encourage our staff to pursue new research directions.

Kimberly S. Budil
LLNL Director

Throughout this year's report, we highlight LDRD's investments in ideas that make the world a safer place. We review key accomplishments and performance indicators and share highlights from projects led by our talented staff. I encourage you to visit our LDRD website and learn more about the 250 projects that we supported during fiscal year 2022.

Finally, while the chronological scope of this report does not include the recent fusion ignition achievement of December 5, 2022, I'd be remiss in failing to mention the magnitude of that accomplishment and the continued role LDRD played in achieving that huge success. Looking to the future, I am confident that LDRD investments will continue to help LLNL remain at the forefront of innovative research and development.

ldrd-annual.llnl.gov

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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 program in 1991 to foster cutting-edge scientific and technical vitality at U.S. Department of Energy (DOE) laboratories. The LDRD programs at each laboratory are 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.

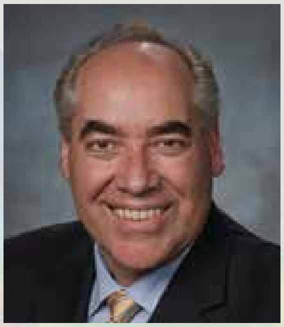
PERFORMANCE ASSESSMENT

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

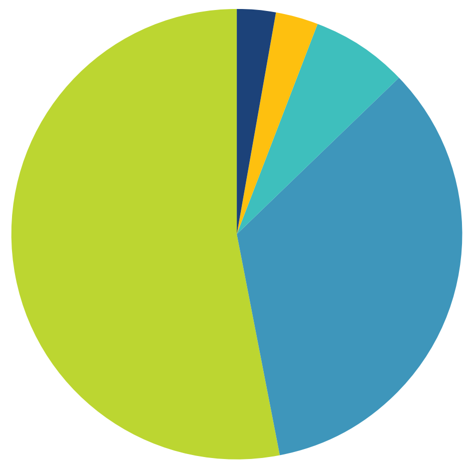
LDRD investments span a broad range of research topics, helping to ensure that LLNL supports innovation in key programmatic areas. Funded projects address some of our newest mission spaces, including cognitive simulation, predictive biology, space science and security, and hypersonic science. We also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

For fiscal year 2022, 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 FY22 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.

Funding by Project Type

Livermore's LDRD program includes five types of projects. Each one has a distinctive purpose, duration, and funding limits. 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.

FY22 INVESTMENTS
250 PROJECTS,
~$138M TOTAL FUNDING



Project Type	FY22 Projects Funded	Project Aim
Exploratory Research	140	Address a specific research challenge or enhance a core competency.
Feasibility Study	37	Determine the viability of a new way to address a mission-relevant challenge.
Lab-wide Competition	37	Conduct innovative basic research and enable out-of-the-box thinking.
Strategic Initiative	19	Make significant progress addressing a mission-relevant challenge from a multidisciplinary perspective.
Disruptive Research	17	Pursue novel ideas with the potential to overturn fundamental paradigms or create new research directions.

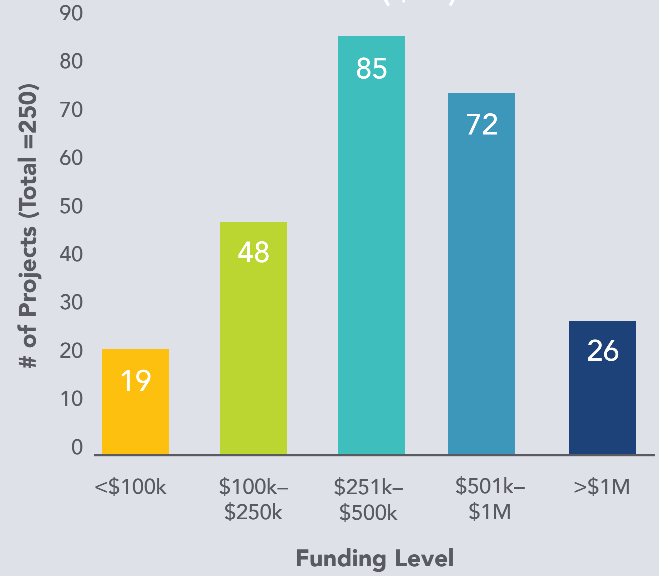
Projects by Funding Level

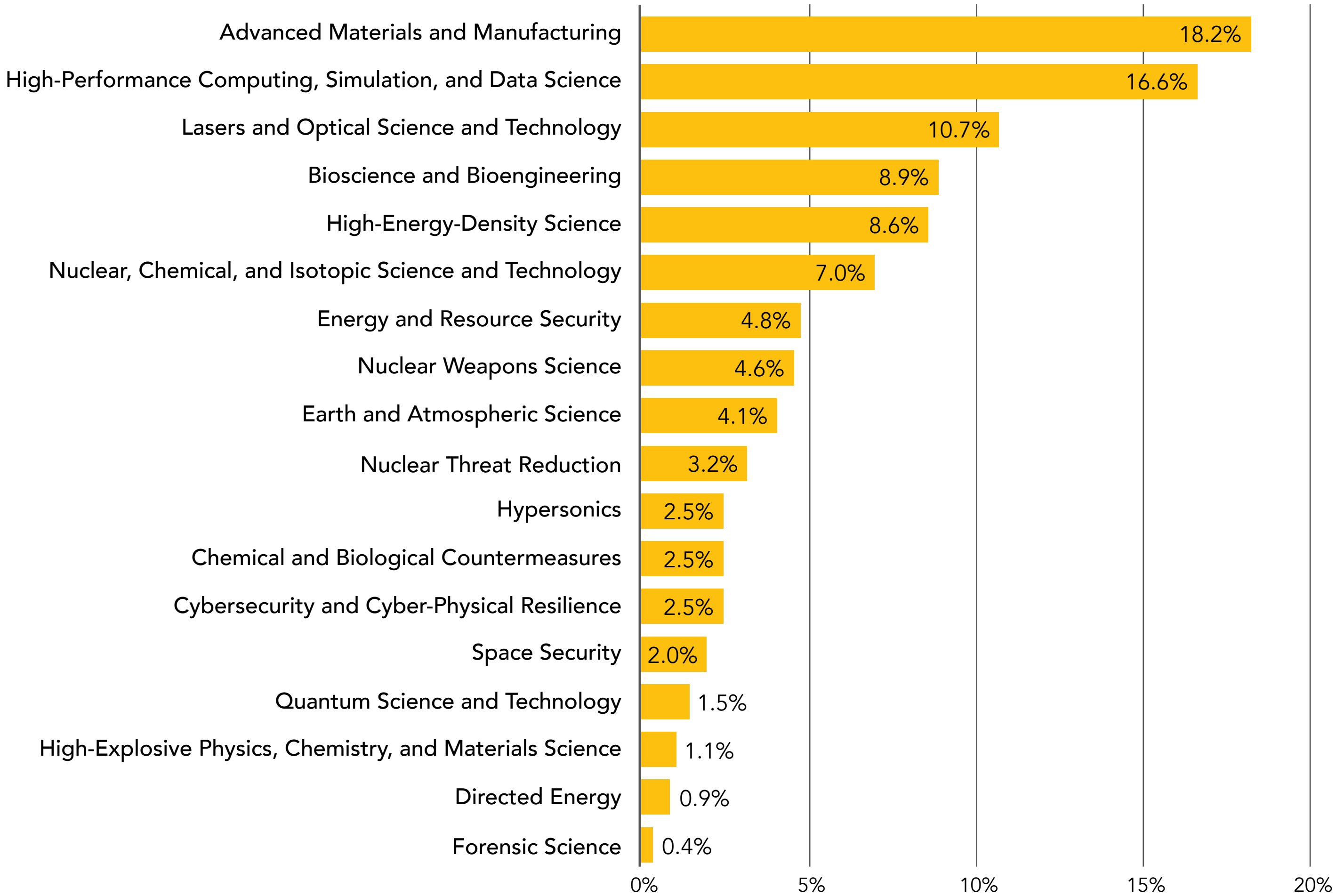
Our Laboratory's investment strategy includes the flexibility to fund projects at varying dollar amounts, depending on the project scope. This chart presents data on the number of projects funded in FY22, distributed across five funding levels. The largest number of projects (85) fell in a higher funding range, receiving between $251k and $500k per project. A smaller number of projects received less than $100k in funding (19 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.)

$553,000 AVERAGE FUNDING LEVEL PER PROJECT ($K)





Program Value

By almost any measuring stick, the LDRD program contributes far more to publications, intellectual property, collaborations, and recruitment of postdoctoral researchers—dollar for dollar—than any other program at the Laboratory.

66 INSTITUTIONS were involved in formal collaborations with LLNL as part of LDRD-funded research teams in FY22.

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 involves 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	FY18	FY19	FY20	FY21	FY22
LDRD-funded projects with one or more formal collaborations	74	74	78	88	79
Percentage of all projects at LLNL	31%	30%	32%	33%	32%

New laser-based volumetric additive manufacturing method can 3D print glass in seconds

Versatile and ubiquitous, glass is increasingly found in specialized applications such as fiber optics, consumer electronics and microfluidics for "lab-on-a-chip" devices. However, traditional glassmaking techniques can be costly and slow, and 3D-printing glass often results in rough textures, making them unsuitable for smooth lenses.

Using a new laser-based Volumetric Additive Manufacturing (VAM) approach — an emerging technology in near-instant 3D printing — researchers at Lawrence Livermore National Laboratory (LLNL) and the University of California, Berkeley have demonstrated the ability to 3D-print microscopic objects in silica glass, part of an effort to produce delicate, layer-less optics that can be built in seconds or minutes. The results are reported in the latest edition of the journal *Science*.

Nicknamed "the replicator" after the fictional device in "Star Trek" that can instantly fabricate nearly any object, the Computed Axial Lithography (CAL) technology developed by LLNL and UC Berkeley is inspired by computed

Lawrence Livermore National Laboratory co-author Caitlyn Krikorian Cook, a group leader and polymer engineer in the Lab's Materials Engineering Division, characterized the curing kinetics of the nanocomposite silica glass resin with light exposure. Photo by Garry McLeod/TID.

Principal Investigator: Maxim Shusteff

LDRD Project: Advanced Photopolymer Materials Engineering for Multiscale Additive Fabrication (19-ERD-012)

tomography (CT) imaging methods. CAL works by computing projections from many angles through a digital model of a target object, optimizing these projections computationally and then delivering them into a rotating volume of photosensitive resin using a digital light projector. Over time, the projected light patterns reconstruct, or build up, a 3D light dose distribution in the material, curing the object at points exceeding a light threshold while the vat of resin spins. The fully formed object materializes in mere seconds — far faster than traditional layer-by-layer 3D printing techniques — and then the vat is drained to retrieve the part.

Combining a new microscale VAM technique called micro-CAL, which uses a laser instead of an LED source, with a nanocomposite glass resin developed by the German company Glassomer and the University of Freiburg, UC Berkeley researchers reported the production of sturdy, complex microstructure glass objects with a surface roughness of just six nanometers with features down to a minimum of 50 microns.

UC Berkeley Associate Professor of Mechanical Engineering Hayden Taylor, the project's principal investigator, said the micro-CAL process, which produces a higher dose of light and cures 3D objects faster and at higher resolution, combined with the nanocomposite resins characterized at LLNL proved a "perfect match for each other," creating "striking results in the strength of the printed objects."

LLNL co-author Caitlyn Krikorian Cook, a group leader and polymer engineer in the Lab's Materials Engineering Division, characterized the curing kinetics of the nanocomposite resin with light exposure. Printing higher-viscosity resins is challenging, if not impossible, with current traditional stereolithography systems at LLNL, according to Cook, and that the benefit of VAM for micro-optics is that it can produce extremely smooth surfaces without layering artifacts, resulting in faster printing without additional post-processing time.

"You can imagine trying to create these small micro-optics and complex microarchitectures using standard fabrication techniques; it's really not possible," Cook said. "And being able to print it ready-to-use without having to do polishing techniques saves a significant amount of time. If you can eliminate polishing steps after forming the optics — with low roughness — you can print a part ready for use."

Cook performed in-situ resin characterization with a spectrometer to measure the thresholding response of an inhibitor modifier in the material's photopolymerization kinetics. The modifier, combined with the preciseness of the laser VAM method, was the "secret sauce" to printing high-resolution optics at a microscale.

"By creating a thresholding response, we're able to significantly improve the resolution," Cook said. "We're taking advantage of the similar thresholding response reported in our previous work, except we're implementing it in a different class of photopolymer chemistry. We're beginning to better understand the necessary kinetics for volumetric manufacturing."

Real-world applications could include micro-optics in high-quality cameras, consumer electronics, biomedical imaging, chemical sensors, virtual-reality headsets, advanced microscopes, and microfluidics with challenging 3D geometries such as "lab-on-a-chip" applications (where microscopic channels are needed for medical diagnostics), fundamental scientific studies, nanomaterial manufacturing and drug screening. Plus, the benign properties of glass lend themselves well to biomaterials, or to cases with high temperature or chemical resistance.

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.

Patents	FY18	FY19	FY20	FY21	FY22
All LLNL patents issued	79	143	200	166	166
LDRD patents issued	41	95	131	96	103
LDRD patents as a percentage of total	52%	66%	66%	58%	62%

LDRD-funded work has played a key role in developing

MORE THAN 50%

of the Laboratory's patents.

Copyrights	FY18	FY18	FY20	FY21	FY22
All LLNL copyrights	105	118	138	125	142
LDRD copyrights	23	24	31	42	47
LDRD copyrights as a per-centage of total	22%	20%	22%	34%	33%

Records of Invention	FY18	FY18	FY20	FY21	FY22
All LLNL records	105	129	126	89	70
LDRD records	47	65	56	53	40
LDRD records as a percent-age of total	45%	50%	44%	60%	57%

LLNL team claims top AI award at international symbolic regression competition

A Lawrence Livermore National Laboratory (LLNL) team claimed a top prize at an inaugural international symbolic regression competition for an artificial intelligence (AI) framework they developed capable of explaining and interpreting real-life COVID-19 data.

Hosted by the open source SRBench project at the 2022 Genetic and Evolutionary Computation Conference (GECCO), the competition had two tracks — synthetic and real-world — and invited teams to submit their best symbolic regression algorithms. Organizers trained the models on datasets, assigned "trust ratings" and evaluated them for accuracy and simplicity.

LLNL computer scientist Brenden Petersen and his team's "Unified Deep Symbolic Regression" (uDSR) algorithm beat out 12 other teams on the real-world track — a task to build an interpretable predictive model for 14-day forecast counts of COVID-19 cases, hospitalizations, and deaths in New York state.

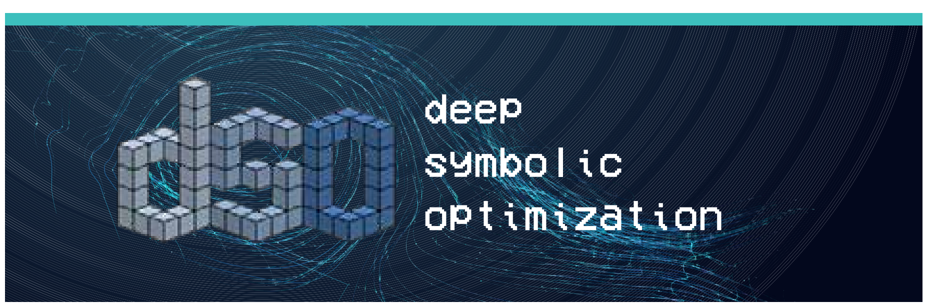
The team's uDSR method is an updated version of their earlier deep symbolic regression algorithm — a reinforcement learning approach using deep neural networks — that finds short mathematical expressions to best fit experimental data and uncovers underlying equations or dynamics of physical processes. The initial framework outperformed previous state-of-the-art baseline methods on benchmark problems. Researchers said the new version unifies deep symbolic regression with four other classes of state-of-the-art symbolic regression algorithms, hybridizing their key capabilities into a single, modular framework.

uDSR is part of a larger framework called Deep Symbolic Optimization (DSO), developed by the team as part of the LDRD. DSO is now being used in several other programs at LLNL: for example, to optimize antibody sequences to bind emerging pathogens.

"This competition is a big win for the Laboratory because our underlying DSO framework is being used for several Lab missions, not just symbolic regression," said Petersen, who serves as the principal investigator on the project. "This victory establishes that we are supporting several Laboratory programs with bleeding-edge technologies of a highly competitive field."

Principal Investigator: Brenden Petersen

LDRD Project: Hypothesis Testing via Artificial Intelligence: Generating Physically Interpretable Models of Scientific Data with Machine Learning (19-DR-003)



LLNL computer scientist Brenden Petersen and team recently claimed first prize in a first-ever international symbolic regression competition for their Unified Deep Symbolic Regression algorithm, based on its exceptional ability to explain and interpret real-life COVID-19 data.

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	FY18	FY19	FY20	FY21	FY22
All LLNL articles	1,178	1,281	1,149	1,256	1,149
LDRD articles	456	553	428	509	490
LDRD articles as a percentage of total	39%	43%	37%	41%	43%

Safe, long-cycle-life batteries with high energy density are greatly needed with the rapid growth of electric devices and vehicles and grid energy storage demands.

Lawrence Livermore National Laboratory (LLNL) scientists have devised a method for the fabrication of all-solid-state lithium metal batteries, which have been recognized as the future choice of safe and high-energy-density power sources.

The team found that sintering (compacting and forming a solid mass of material by heat or pressure without melting it to the point of liquefaction) the solid-state electrolyte films with carbon dioxide (CO2) overcomes the common manufacturing challenges in solid-state batteries.

The laser sintering technique yields scalable, low-cost, high-energy-density solid-state lithium (Li) batteries that can advance energy storage needs across national security missions. These laser-based techniques also can be applied to other fields, such as additive manufacturing of polymers, ceramics, and metals.

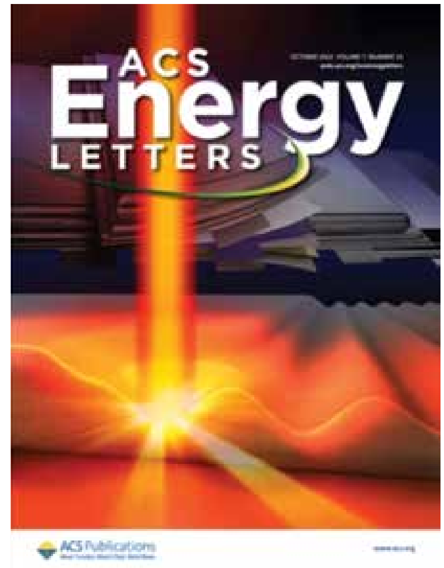
Typical Li-ion batteries (LIBs) use organic liquid electrolytes and graphite anodes, which lead to safety hazards and lower the energy density. Among the various substitutes, all-solid-state Li-metal batteries — with the integration of solid-state electrolytes (SSEs) — are foreseen as the next generation of energy-storage devices that not only effectively address battery safety concerns, but also enable the utilization of Li metal anodes

Principal Investigator: Jianchao Ye

LDRD Project: Laser Processing of Solid State Lithium Batteries (20-ERD-018)

and high-capacity/high-voltage cathode materials to achieve higher energy density.

"This work provides a unique, scalable and widely applicable ultrarapid laser sintering technique to overcome the difficulties associated with classic methods for the integration of SSEs for practical solid-state Li-metal battery applications," said LLNL materials scientist Jianchao Ye, corresponding author of a paper appearing on the cover of *ACS Energy Letters*.



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	FY18	FY19	FY20	FY21	FY22
Students supported by LDRD	138	160	101	136	149
Percentage of all students	22%	23%	18%	24%	23%

Postdoctoral Researchers	FY18	FY19	FY20	FY21	FY22
Postdoctoral researchers supported by LDRD ≥10% of their time	167	170	208	208	240
Percentage of all postdoctoral researchers	54%	57%	63%	54%	56%
LDRD postdoctoral researchers converted to full staff	52	46	60	50	72
Percentage of all conversions	71%	68%	77%	82%	77%

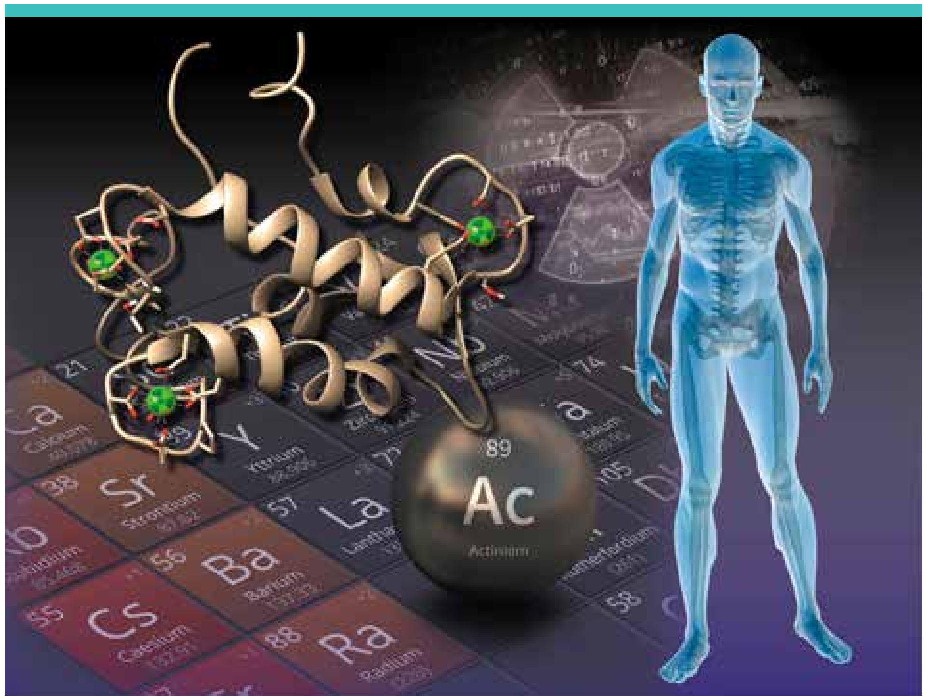
Cancer therapies and nuclear material detection get a boost from newly discovered protein

Lawrence Livermore National Laboratory (LLNL) and Penn State scientists have demonstrated how a protein can be recovered and purified for radioactive metals like actinium that could be beneficial for both next-generation drugs used in cancer therapies and the detection of nuclear activities.

Radioactive metals hold unique and essential places in a variety of medical imaging and therapeutic applications, but they require lengthy separation processes for their purification as well as synthetic and costly chelators (molecules tailored to bind the radioactive metal ions) that must form exceptionally stable complexes in the patient to minimize toxicity.

Principal Investigator: Gauthier DeBlonde

LDRD Project: Elusive Actinium: A First Glimpse into the Coordination Chemistry of Element 89 (20-LW-017)



Actinium is a radioactive element that could revolutionize cancer medicine, but its chemistry has thus far remained elusive. LLNL and Penn State researchers developed a new approach to study, capture and purify medical isotopes, including actinium. Their strategy leverages a natural protein that can tightly bind to medical isotopes without interacting with process impurities like radium, strontium, etc. Artwork by Thomas Reason/LLNL

Actinium-based therapies could revolutionize cancer medicine, with treatment efficacy hundreds of times higher than current drugs. However, they remain out of reach due to difficulties throughout the actinium supply chain, from isotope production to studying the element's chemistry, and development of robust chelators for it.

"These challenges exist even for medical isotopes in relatively widespread use, such as radioactive yttrium, but they are even more taxing in the case of actinium," said LLNL scientist Gauthier DeBlonde, a Post-Doc at LLNL and lead author of a paper appearing in Science Advances.

As it turns out, actinium is one of the rarest elements naturally occurring on Earth, and its medical isotope must be produced in nuclear reactors or other large and costly instruments. As such, actinium chemistry is among the least understood and this impedes the development actinium-based medical applications. Research efforts have thus far focused on reusing or adapting known synthetic molecules used in the nuclear chemistry field, but results have been limited with actinium. The new research took a drastically new approach and leveraged a natural protein, lanmodulin, discovered by the Penn State members of the team in 2018. This new strategy not only improves and simplifies the purification processes for actinium but can also be used to recover and detect other radioactive elements, even at extremely low levels.

The team showed how lanmodulin can be used to bind, recover, and purify actinium (at least 99.5 percent purity obtained in a single step), as well as another medically relevant radioisotope, yttrium-90, which is used for cancer therapy and diagnostics. The unprecedented efficiency and simplicity of the protein-based approach also allows preparation of actinium at much lower cost and probing its chemistry more conveniently. The process also is likely extendable to many other radioactive isotopes used in radiation therapy and imaging.

"Our new technique represents a paradigm shift not just in the development of actinium chemistry and actinium-based pharmaceuticals, but also in nuclear medicine more generally," said Joseph Cotruvo Jr., co-corresponding author, and Penn State assistant professor of chemistry.

The actinium-lanmodulin complex is the very first actinium protein to be characterized. The researchers found that lanmodulin is so efficient compared to classic molecules that it specifically binds actinium even in the presence of large quantities of process impurities, like radium and strontium, or physiological elements like calcium, zinc, copper, etc. The study also demonstrates that the protein is more effective at binding actinium than binding the rare earth elements, the metals it binds to in nature.

DeBlonde said, "What we accomplished here was simply unfathomable a few years ago. The unique combination of skills in radiochemistry, metal separation and biochemistry at LLNL and Penn State made this possible. I believe our technology will be incredibly useful not only to nuclear medicine but also for the in-field analysis of radioactive samples."

Professional Fellows

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 2022, 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.

HISTORY OF APS FELLOWS AT LLNL

	Single-Year Statistics			Multi-Year Statistics		
	FY20	FY21	FY22	FY13–17	FY18–22	FY13–22
Total APS awards	4	3	2	30	19	49
Awards with LDRD roots	4	3	2	29	18	47
% with LDRD roots	100%	100%	100%	97%	95%	96%
Average years from first LDRD experience	20.8	8	15	14.8	15.9	15.2

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.

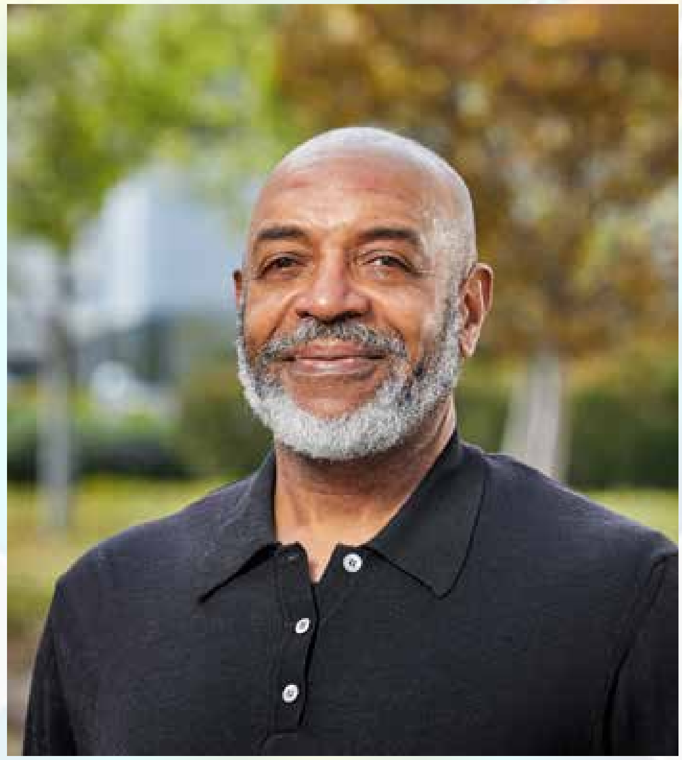
2022 APS Fellows at LLNL

Two LLNL scientists were selected as 2022 fellows of the American Physical Society. The new fellows were both selected by the APS Division of Plasma Physics.

ANNIE KRITCHER

"I am extremely honored to be receiving this award. This is one of the most important awards I will achieve in my career and I'm grateful to have been chosen to become an APS Fellow."

Annie Kritcher, a physicist in the Weapons and Complex Integration's Design Physics Division, was selected "for leadership in integrated hohlraum design physics leading to the creation of the first laboratory burning and igniting fusion plasma." Annie is a team lead within the Inertial Confinement Fusion (ICF) program, where she oversees the integrated modeling of indirect-drive fusion designs fielded at the NIF.



RONNIE SHEPHERD

"I am honored at being elected an APS-DPP fellow. The honor is a recognition of all the hard work of those that have helped develop the LLNL ultrafast X-ray streak camera, analyze the data, and perform simulations to interpret the physics. I owe them all a great debt of gratitude."

A 38-year veteran, Shepherd serves as the director of outreach at the High Energy Density Science Center. His work focuses on experimental studies of atomic processes in high-density plasmas. The experiments are performed using ultrafast X-ray spectroscopy of short-pulse, laser-heated solids.

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 2022, 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.

HISTORY OF DMTS AWARDS AT LAWRENCE LIVERMORE NATIONAL LABORATORY

	Single-Year Statistics			Multi-Year Statistics		
	FY20	FY21	FY22	FY13-17 (5 yrs)	FY18-22 (5 yrs)	FY13-22 (10 yrs)
Total DMTS awards	0	0	26	24	36	60
DMTS with LDRD roots	N/A	N/A	23	21	33	54
% with LDRD roots	N/A	N/A	89%	88%	92%	90%
Average years from first LDRD experience	N/A	N/A	20	14.0	19.3	17.3

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 on the following page, 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.

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 35% 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

	Single-Year Statistics			Multi-Year Statistics		
	FY20	**FY21**	**FY22**	**FY13-17 (5 yrs)**	**FY18-22 (5 yrs)**	**FY13-22 (10 yrs)**
Total R&D 100 awards	1	3	3	22	11	33
Awards with LDRD roots	0	0	2	8	4	12
% with LDRD roots	0%	0%	67%	36%	36%	36%
Average years from first LDRD investment	N/A	N/A	7.5	6.9	9.8	7.8

THE RENOWNED R&D 100 COMPETITION, NOW IN ITS 60TH YEAR, RECEIVED ENTRIES FROM 17 COUNTRIES AND REGIONS AROUND THE WORLD.

R&D 100 AWARDS

Two LDRD-Funded Projects Win R&D 100 Awards in 2022

Two of LLNL's three R& D 100 Awards – for Energy Inks and Tailored Glass by Direct Ink Writing – received internal funding from the Laboratory Directed Research and Development (LDRD) Program.

The Laboratory has now collected a total of 176 R&D 100 awards since 1978. Energy Inks and Tailored Glass by Direct Ink Writing — received internal "seed money" from the Laboratory Directed Research and Development (LDRD) program. This funding enables undertaking high-risk, potentially high-payoff projects at the forefront of science and technology.

This year's LLNL R&D 100 awards include an additive manufacturing process called Tailored Glass by Direct Ink Writing that prints silica-based optics and glass components into customizable forms, novel compression gratings that enable a new class of high-energy laser systems, and a three-dimensional printing feedstock known as Energy Inks that can print a functioning battery.

"It is a great tribute to the innovative spirit of our scientists and engineers to be selected for an R&D 100 award," Lab Director Kim Budil said. "Teaming with industrial collaborators is an important element in ensuring that the transformative technologies developed at LLNL will benefit the nation."

The Tailored Glass team is led by chemical engineer Rebecca Dylla-Spears and includes physicists Du Nguyen and Michael Johnson; materials scientists Jungmin Ha, Timothy Yee and Becca Walton; chemists Koroush Sasan and Tyler Fears; chemical engineer Nikola Dudukovic; mechanical engineer Megan Ellis; and optical engineer Oscar Herrera.

Lab scientists and engineers have developed Energy Inks, a three-dimensional (3D) printer feedstock that allows the production of a functioning battery and other devices. 3D printing with polymers allows a newer and more efficient method of prototyping. Now Energy Inks, which have functional properties, are optimized to enable next-generation, high-performance 3D-printed devices for energy storage, catalysis, filtration, sensors, and more uses.

Materials scientist Swetha Chandrasekaran and chemical engineer Marcus Worsley, team leaders of the Energy Links team, and Rebecca Dylla-Spears, chemical engineer and leader of the Tailored Glass team, earned R&D100 Awards.

The LLNLteam that developed Energy Inks received funding through a Department of Energy Technology Commercialization Fund grant. It is led by materials scientist Swetha Chandrasekaran and chemical engineer Marcus Worsley.

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 250 projects in fiscal year 2022. Brief summaries of each project are included in the Project Highlights section of our online report at ldrd-annual.llnl.gov. Here, we provide a closer look at a handful of projects that underscore the exciting, innovative research in this year's LDRD portfolio.

Research finds mechanically driven chemistry accelerates reactions in explosives

Scientists at the Lawrence Livermore National Laboratory (LLNL) Energetic Materials Center and Purdue University Materials Engineering Department used simulations performed on the LLNL supercomputer Quartz to uncover a general mechanism that accelerates chemistry in detonating explosives critical to managing the nation's nuclear stockpile. Their research is featured in the July 15 issue of the *Journal of Physical Chemistry Letters*.

Insensitive high explosives based on TATB (1,3,5-triamino-2,4,6-trinitrobenzene) offer enhanced safety properties over more conventional explosives, but physical explanations for these safety characteristics are not clear. Explosive initiation is understood to arise from hotspots that are formed when a shockwave interacts with microstructural defects such as pores. Ultrafast compression of pores leads to an intense localized spike in temperature, which accelerates chemical reactions needed to initiate burning and ultimately detonation. Engineering models for insensitive high explosives — used to assess safety and performance — are based on the hotspot concept but have difficulty in describing a wide range of conditions, indicating missing physics in those models.

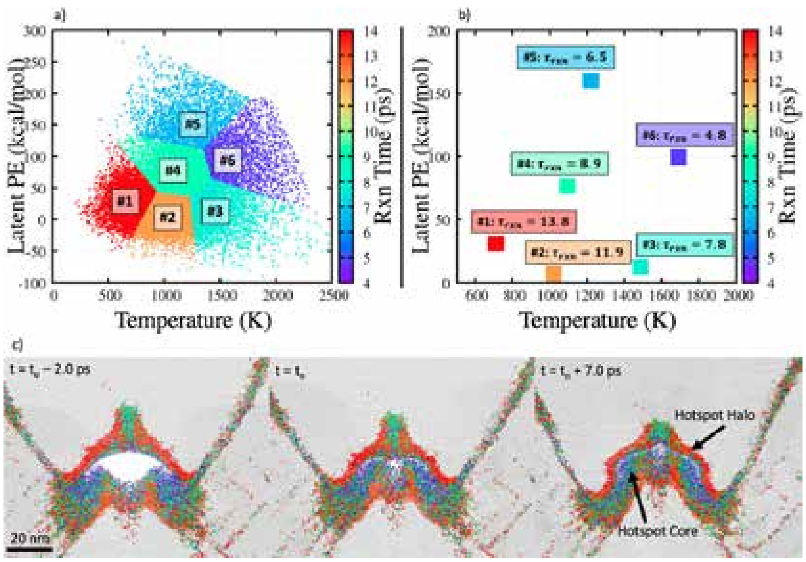
Using large-scale atomically resolved reactive molecular dynamics supercomputer simulations, the team aimed to directly compute how hotspots form and grow to better understand what causes them to react.

Chemical reactions generally accelerate when the temperature is increased, but there are other potential mechanisms that could influence reaction rates.

"Recent molecular dynamics simulations have shown that regions of intense plastic deformation, such as shear bands, can support faster reactions," explained LLNL author Matthew Kroonblawd. "Similar accelerated rates also were observed in the first reactive molecular dynamics simulations of hotspots, but the reasons for the accelerated reactions in shear bands and hotspots were unclear."

The main advantage and predictive power of molecular dynamics simulations come from their complete resolution of all the atom motions during a dynamic event.

"These simulations generate enormous quantities of data, which can make it difficult to derive general physical insights for how atom motions govern the collective material response," said Ale Strachan of Purdue University.



Molecular descriptors (a) and cluster centroids (b) colored by τrxn plotted in T–Ulatent space. (c) Spatial mapping of clustered molecules about the hotspot during and after its formation. Molecules are colored by cluster ID following the convention in panels a and b, with nonclustered molecules colored white.

Principal Investigator: Lara Leininger

LDRD Project: Unlocking the Mysteries of High-Explosive Science (18-SI-004)

To better grapple with this big data problem, the team turned to modern data analytic techniques. Through clustering analysis, the team found that two molecular state descriptors were connected to chemical reaction rates. One of these is the temperature, which is well-understood from traditional thermochemistry. The other important descriptor is a newly proposed metric for the energy associated with deformations of molecule shape, that is, the intramolecular strain energy.

The team's clustering analysis revealed that molecules in a hotspot that are driven from their equilibrium planar shape react more quickly; mechanical deformations of molecules in regions of intense plastic material flow lead to a mechanochemical acceleration of rates.

Mechanically driven chemistry (mechanochemistry) is known to operate in many systems, ranging from precision manipulation of bonds through atomic force microscopy "tweezers" to industrial-scale ball milling.

The mechanochemistry that operates in shocked explosives is not directly triggered, but results from a complicated cascade of physical processes that start when a shock induces plastic material deformations.

The work provides clear evidence that mechanochemistry of deformed molecules is responsible for accelerating reactions in hotspots and in other regions of plastic deformation, such as shear bands.

"This work provides a quantitative link between hotspot ignition chemistry and the recent 2020 LLNL discovery of shear band ignition, which provides a firm basis for formulating more general physics-based explosive models," Kroonblawd said. "Including mechanochemical effects in explosives models will improve their physical basis and allow for systematic improvements to assess performance and safety accurately and reliably."

Researchers design a new plasma optics for the development of high-power compact lasers

Lawrence Livermore National Laboratory (LLNL) researchers have designed a compact multi-petawatt laser that uses plasma transmission gratings to overcome the power limitations of conventional solid-state optical gratings. The design could enable construction of an ultrafast laser up to 1,000 times more powerful than existing lasers of the same size.

The new design could make it possible to field a laser system similar in size to the LLNL-designed L3 HAPLS (High-Repetition-Rate Advanced Petawatt Laser System) at ELI Beamlines in the Czech Republic, but with 100 times the peak power.

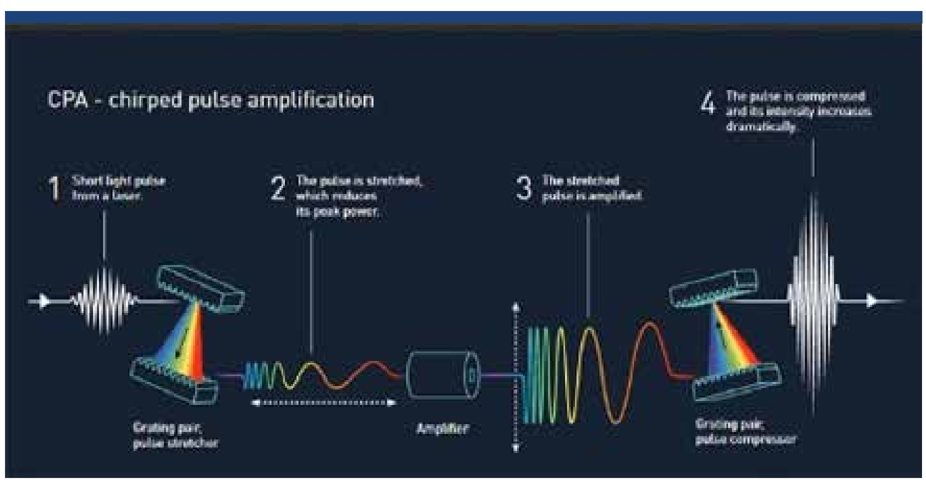
Petawatt (quadrillion-watt) lasers rely on diffraction gratings for chirped-pulse amplification (CPA), a technique for stretching, amplifying, and then compressing a high-energy laser pulse to avoid damaging optical components. CPA, which won a Nobel Prize in physics in 2018, is at the heart of the National Ignition Facility's Advanced Radiographic Capability as well as NIF's predecessor, the Nova Laser, the world's first petawatt laser

With a damage threshold several orders of magnitude higher than conventional reflection gratings, plasma gratings "allow us to deliver a lot more power for the same size grating," said former LLNL postdoc Matthew Edwards, co-author of a *Physical Review Applied* paper describing the new design published online. Edwards was joined on the paper by Laser-Plasma Interactions Group Leader Pierre Michel.

"Glass focusing optics for powerful lasers must be large to avoid damage," Edwards said. "The laser energy is spread out to keep local intensity low. Because the plasma resists optical damage better than a piece of glass, for example, we can imagine building a laser that produces hundreds or

Principal Investigator: Matthew Edwards

LDRD Project: LDRD Project: Ultrafast Plasma Optics for High-Power Coherent Light Sources (20-ERD-057)



New caption: The chirped-pulse amplification technique makes it possible for a petawatt laser's high-power pulses to pass through laser optics without damaging them. Before amplification, low-energy laser pulses are passed through diffraction gratings to stretch their duration by as much as 25,000 times. Thus, their peak power is reduced and optics that the pulses pass through remain intact. After amplification, the pulses are recompressed back to near their original duration. Credit: The Nobel Committee for Physics.

thousands of times as much power as a current system without making that system bigger."

LLNL, with 50 years of experience in developing high-energy laser systems, also has been a longtime leader in the design and fabrication of the world's largest diffraction gratings, such as the gold gratings used to produce 500-joule petawatt pulses on the Nova laser in the 1990s. Still larger gratings, however, would be required for next-generation multi-petawatt and exawatt (1,000-petawatt) lasers to overcome the limits on maximum fluence (energy density) imposed by conventional solid optics (see "Holographic Plasma Lenses for Ultra-High-Power Lasers").

Edwards noted that optics made of plasma, a mixture of ions and free electrons, are "well suited to a relatively high-repetition-rate, high-average-power laser." The new design could, for example, make it possible to field a laser system similar in size to the L3 HAPLS (High-Repetition-Rate Advanced Petawatt Laser System) at ELI Beamlines in the Czech Republic, but with 100 times the peak power.

Designed and constructed by LLNL and delivered to ELI Beamlines in 2017, HAPLS was designed to produce 30 joules of energy in a 30-femtosecond (quadrillionth of a second) pulse duration, which is equal to a petawatt, and do so at 10 Hertz (10 pulses per second).

"If you imagine trying to build HAPLS with 100 times the peak power at the same repetition rate, that is the sort of system where this would be most suitable," said Edwards, now an assistant professor of mechanical engineering at Stanford University.

"The grating can be remade at a very high repetition rate, so we think that 10 Hertz operation is possible with this type of design. However, it would not be suitable for a high-average-power continuous-wave laser."

"We're aiming for a design where that kind of inhomogeneity is as small a problem as possible for the overall system —the design should be very tolerant to imperfections in the plasma that you use."

Research reveals where carbon storage has the most potential in soils

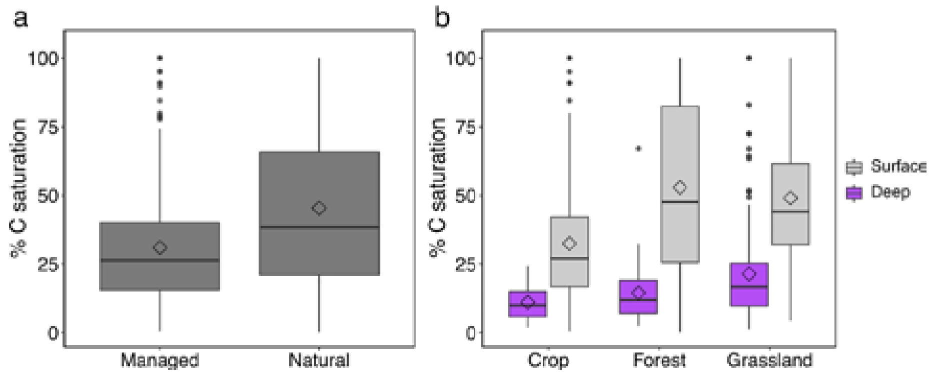
Soil is the largest terrestrial reservoir of organic carbon and is central for climate change mitigation and adaptation. Mineral-organic associations play a critical role in soil carbon preservation, but the global capacity for storage in this form has never been quantified.

New research from Lawrence Livermore National Laboratory (LLNL) and an international team of collaborators addresses this gap by producing the first spatially resolved global estimates of mineral-associated carbon and the carbon-storage capacity of soil minerals.

The research — led by LLNL Lawrence fellow Katerina Georgiou, and appearing in *Nature Communications*— gathered measurements from 1,144 globally-distributed soil profiles to better understand the role of climate and management on driving current mineral-associated carbon stocks and the departure of soils from their mineralogical capacity.

Principal Investigator: Katerina Georgiou

LDRD Projects: LDRD Project From Microbes to the Earth System – Upscaling Microbial Community Dynamics to Macro-scale Soil Carbon Models (21-ERD-045)



Percent mineralogical carbon saturation across ecosystems and soil depths.

The study found that regions under agricultural management and deeper soil layers contain the largest undersaturation of mineral-associated carbon; the degree of undersaturation can help inform sequestration efficiency over years to decades.

The team showed that across 103 carbon accrual measurements spanning management interventions globally, soils furthest from their mineralogical capacity are more effective at accruing carbon. Sequestration rates average three times higher in soils at one tenth of their capacity compared to soils at one half of their capacity.

Soil organic carbon is an integral component of terrestrial ecosystems and plays an important role in ecosystem resilience and productivity. Over the last two centuries, human land-use and land-cover change have resulted in a significant net loss of soil carbon.

"Improved soil management practices that promote soil carbon sequestration, especially in stable carbon pools, are needed to reverse this trajectory and help mitigate climate change," said Georgiou, lead author of the paper.

"Our findings provide insights into the world's soils, their capacity to store carbon and priority regions and actions for soil carbon management," she added.

Oxygen effects on uranium tested

A team of researchers from Lawrence Livermore National Laboratory (LLNL) and the University of Michigan has found that the rate of cooling in reactions dramatically affects the type of uranium molecules that form.

The team's experimental work, conducted over about a year-and-a-half starting in October 2020, attempts to help understand what uranium compounds might form in the environment after a nuclear event. It has recently been detailed in *Scientific Reports*, a *Nature*-affiliated publication.

"One of our most important findings was learning that the rate of cooling affects the behavior of uranium," said Mark Burton, the paper's lead author and a chemist in the Lab's Materials Science Division. "The big picture here is that we want to understand uranium chemistry in energetic environments."

Lab researchers Mark Burton (front right) and Jonathan Crowhurst align the laser ablation chamber for in-situ analysis of uranium oxide particulates. Photo by Julie Russell, LLNL

Principal Investigator: Kimberly Knight

LDRD Project: LDRD Project: Identifying the Influence of Environmental Effects on Post-Detonation Chemistry and Debris Formation (20-SI-006)

In their experiments, the LLNL and Michigan researchers found that the rate of cooling — as well as the amount of oxygen — dramatically affect how uranium combines with oxygen.

The recent experiments showed that as uranium cools from a plasma at about 10,000 degrees Celsius in microseconds (millionths of a second), the chemistry is drastically different when compared to cooling over milliseconds (thousandths of a second).

The most recent work, performed under a Laboratory Directed Research and Development (LDRD) strategic initiative, seeks to understand the effect of the local environment on the physics and chemistry of nuclear explosions, particularly to aid computational modeling efforts.

"The electron structures of actinides, such as uranium and plutonium, are extremely complex and difficult to computationally model," said Kim Knight, a co-author of the study and the leader of the LDRD strategic initiative.

"Experiments like this one can provide data and insight on the generalized behavior of these actinides, something that aids our computational modeling."

Uranium and oxygen can combine to form hundreds of different molecules, depending on the oxygen concentration and the cooling rates; each of these species can have different and distinct chemical behaviors.

"When uranium comes into contact with oxygen, it will form different molecules. The rate of cooling also affects the type of molecules that form. We care about what specific molecules are formed as a result," Burton explained.

"These experiments improve our understanding of gas-phase chemical reactions between uranium and oxygen as hot plasmas cool, which can inform models of nuclear explosions to refine our predicative capabilities of particle formation and transport," Knight said.

"The fate of uranium in the environment is important for predicting the impact of events like nuclear weapons or nuclear accidents in different environments. One of the applications is to aid in the interpretation of events for nuclear forensics," she added.

Breaking the strongest chemical bonds with laser shock compression

Lawrence Livermore National Laboratory (LLNL) scientists recently obtained high-precision thermodynamic data on warm dense nitrogen at extreme conditions that could lead to a better understanding of the interiors of celestial objects like white dwarfs and exoplanets.

The team, which includes researchers from the University of California, Berkeley and the University of Rochester, used an advanced technique that combines pre-compression in a diamond anvil cell and laser-driven shock compression at the Omega Laser Facility at the University of Rochester.

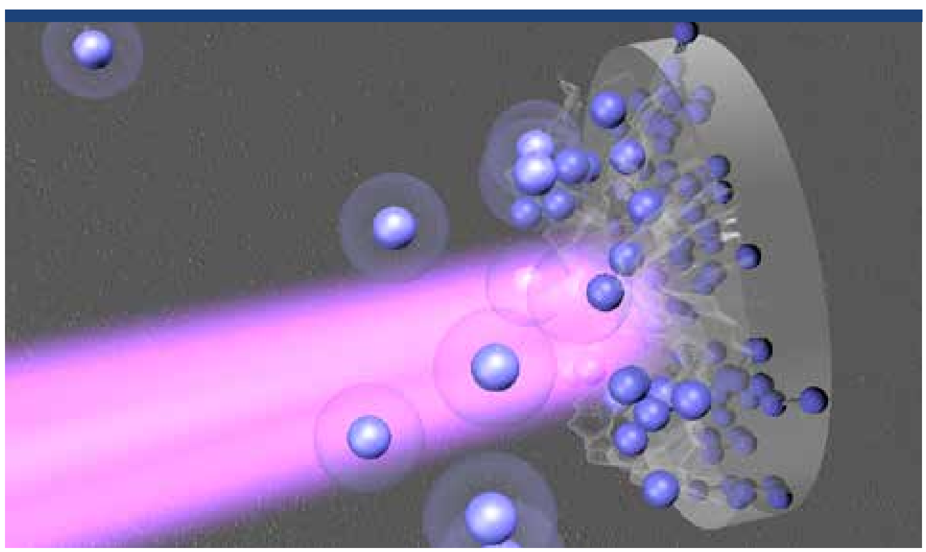
Molecules of nitrogen (N2) make up 78% of the air we breathe. They are unique because the two nitrogen atoms in N2 are bound with a triple covalent bond, which is the strongest of all simple diatomic molecules. Nitrogen also is an important constituent of celestial bodies in the outer solar system and beyond. For example, ammonia (NH3) storms are believed to exist in giant planets like Jupiter, while the dwarf planet Pluto, Saturn's icy moon Titan and Neptune's icy moon Triton have N2-rich atmospheres.

Previous studies with this powerful technique revealed experimental evidence for superionic water ice and helium rain in gas-giant planets. In the new research, the team conducted shock experiments on precompressed molecular nitrogen fluid up to 800 GPa (~8 million atmospheres) of pressure.

They observed clear signatures for the completion of molecular dissociation near 70-100 GPa and 5-10 kK (thousands of kelvins) and the onset of ionization for the outermost electrons above 400 GPa and 50 kK.

Principal Investigator: Marius Millot

LDRD Projects: LDRD Project: Unraveling the Physics and Chemistry of Water-Rich Mixtures at Extreme Pressures and Temperatures (19-ERD-031)



Laser-driven shock waves reaching several million atmospheres break the extremely strong triple-bond of nitrogen molecules and free up a fraction of the L-shell electrons of the dissociated atoms. Image by Liam Krauss/LLNL.

"It is very exciting that we can use shock waves to break these molecules and understand how pressure and density induce changes in chemical bonding," said LLNL physicist Yong-Jae Kim, lead author of a paper appearing in *Physical Review Letters*.

"Studying how to break nitrogen molecules and how to free up electrons is a great test for the most advanced computer simulations and theoretical modeling."

The team also theorized that studying nitrogen might help to unlock some of the mysteries regarding the behavior of hydrogen molecules in the early stage of inertial confinement fusion implosions at the National Ignition Facility.

"While nitrogen and hydrogen are both light diatomic molecules, hydrogen atoms are so small that reproducing their behavior under extreme pressure and temperature with computer simulations is very complex," Kim said.

The team took a closer look at the comparison between the experimental data in the new research and the corresponding simulated pressure-density curves starting from different initial densities. The comparison provided further confidence in the ability of computer simulations using the density functional theory (DFT) molecular dynamics technique to accurately capture the subtle quantum physics changes in material properties at these previously undocumented conditions. In particular, the new data resolved a puzzling discrepancy between previous experiments on warm dense nitrogen and predictions based on the results of the DFT simulations.

The research is part of a Laboratory Directed Research and Development (LDRD) project to develop new laser-driven dynamic compression experimental techniques with diamond anvil cell (DAC) targets. These techniques could unravel new physics and chemistry phenomena in low atomic-number mixtures, such as those rich in water, over a wide range of unprecedented pressure-temperature-density conditions. The research has implications for planet formation and evolution and provide insights into the properties of matter under extreme conditions.

LLNL study on tumor/immune cell interaction could impact cancer immunotherapies

Lawrence Livermore National Laboratory (LLNL) scientists exploring the interaction between cancer cells and the extracellular matrix (ECM) — the "scaffolding" of organs — found that proteins in the ECM can dramatically impact the immune system's ability to kill tumors. Researchers said the findings, published online in the journal *Biomaterials*, could represent a novel approach to studying immunosuppression found in many breast cancers and open new pathways of activating the immune system to target cancer.

In the paper, LLNL engineers and biologists report on the development of an assay for testing the efficacy of T cells — the white blood cells that in healthy persons surveil and eliminate precancerous cells. But in most breast cancers, these T cells fail to do their job.

The researchers cultured tumor and immune cells on various compositions of ECM (the molecules and proteins that make up the structural support system surrounding cells). By screening 25,000 cells on 36 different combinations of nine ECM proteins, the team demonstrated, for the first time, the ability of immune cells to clear tumors is regulated by the makeup of the ECM substrate.

"The surprising thing was finding the ability of the immune cell to kill a tumor depends on what [scaffolding proteins] the tumor is sitting on," said LLNL mechanical engineer Claire Robertson, who led the work. "Depending on the ECM environment, the tumor cells were either completely susceptible and died off or they remained completely resistant to T cells."

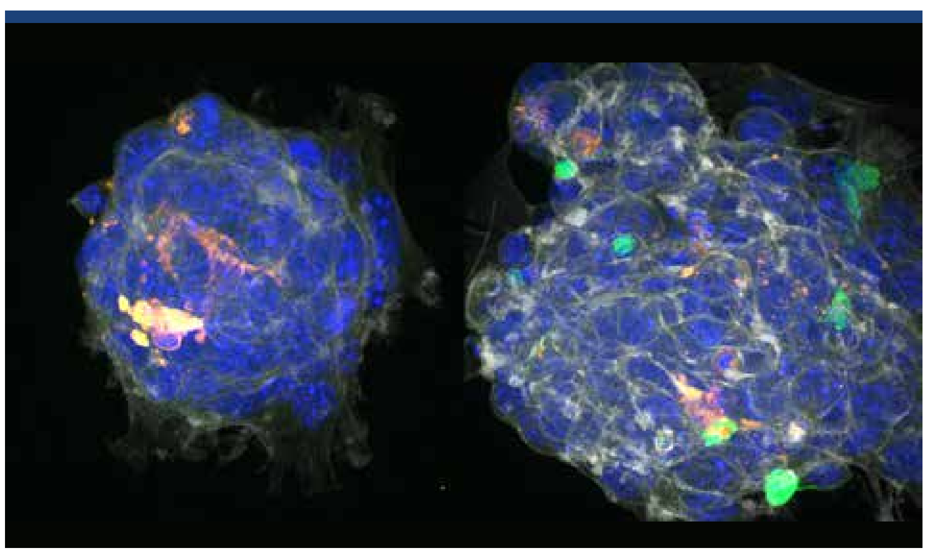
Most notably, the team found that in the presence of Collagen IV, breast cancer cells were more likely to grow and were more resistant to T cells, whereas T cells were more likely to die off. "The T cells that were touching Collagen IV were just not doing their job," Robertson said. "In fact, we found that any time Collagen IV was in the mix, the T cells were dying instead of the tumor cells — exactly what you don't want to happen if you have a tumor."

Researchers also discovered that in Collagen IV, T cells turned off gene signatures related to killing harmful cells, whereas tumor cells turned on signatures of cytokines that send messages to T cells that there is no tumor present.

Robertson said the experimental results provide clues as to why immune checkpoint therapies like Programmed death-ligand 1 (PD-L1) inhibitors, which have improved the prognosis of various cancers, have been largely ineffective in treating breast cancer. Breast cancers rarely express PD-L1 development as biomarkers, making patients ineligible for such therapies, she explained. Importantly, tumor cells cultured on Collagen IV turned PD-L1 off, but still showed profound immunosuppression, mimicking what happens in human breast tumors, Robertson added.

Principal Investigator: Elizabeth Wheeler

LDRD Projects: Engineered and Instrumented Three-Dimensional Tumor-Immune Model System (19-SI-003)



Left: This image shows tumor and immune cells (blue for all nuclei) grown on Collagen IV. The orange spots show T-cells (immune cells) in the process of dying. Right: This image depicts tumor cells combined with living T-cells growing on a scaffolding of proteins. Images courtesy Monica Moya/LLNL.

"The question is, what can we do to activate the immune system in these patients? The thing that's really exciting is the fact that we've found a completely unique mechanism of immunosuppression. It means we have a whole new way of targeting cancer," she said.

Researchers said the pipeline they developed could apply beyond breast cancer to nearly any form of cancer.

"This research offers a new approach to identify and tease apart the critical components for understanding the biology of tumors, which may provide novel insight for more targeted cancer treatment," said co-author Matt Coleman, a Translational Immunobiology group leader in the Lab's Biosciences & Biotechnology Division.

Where on Earth did the water come from?

Earth's supply of water is incredibly important for its ability to sustain life, but where did that water come from? Was it present when Earth formed or was it delivered later by meteorites or comets from outer space?

The source of Earth's water has been a longstanding debate and Lawrence Livermore National Laboratory (LLNL) scientists think they have the answer — and they found it by looking at rocks from the moon.

Since the Earth-moon system formed together from the impact of two large bodies very early in solar system history, their histories are very much linked. And since the moon lacks plate tectonics and weathering, processes that tend to erase or obscure evidence on Earth, the moon is actually a great place to look for clues to the history of Earth's water.

Even though close to 70 percent of Earth's surface is covered with water, overall, the planet is a relatively dry place compared to many other objects in the solar system. And the moon is even drier. Conventional wisdom was that the lack of volatile species (such as water) on the Earth — and particularly the moon — was due to this violent impact that caused depletions in volatile elements.

But by looking at the isotopic makeup of lunar rocks, the team found that bodies involved in the impact that formed the Earth-moon system had very low levels of volatile elements prior to the impact, not because of it. Specifically, the team used the relative amount of the volatile and radioactive isotope rubidium-87 (87^{Rb}), which is calculated from its daughter isotope strontium-87 (87Sr), to determine the budget of Rb in the Earth-moon system when it formed. The team found that because 87Sr, a proxy for the moon's long-term volatile budget, was so low the bodies that collided must have both been dry to start with, and not much could have been added since.

"Earth was either born with the water we have, or we were hit by something that was basically pure H_2O, with not much else in it. This work eliminates meteorites or asteroids as possible sources of water on Earth and points strongly toward the 'born with it' option," said cosmochemist Greg Brennecka, a co-author of the paper.

In addition to greatly narrowing the potential source of Earth's water, this work additionally reveals that the large bodies that collided must have both come

Principal Investigator: Gregory Brennecka

LDRD Project: Addressing Unresolved Questions About the Solar System with New Lunar Samples from the Apollo Missions (20-ERD-001)

Evidence from the analysis of lunar samples suggest that although the Earth and moon formed from a giant impact, they mostly retained their primordial abundances of volatile elements, including water. Image by Adam Connell/LLNL.

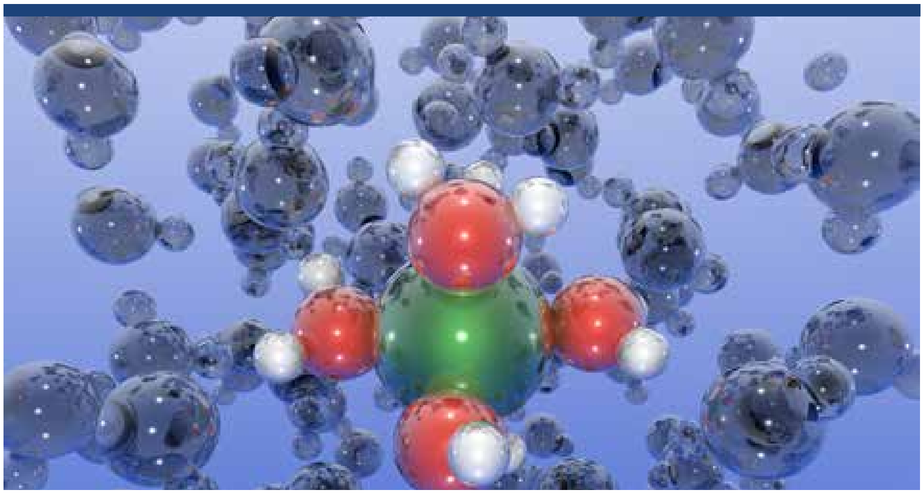
from the inner Solar System, and the event could not have happened prior to 4.45 billion years ago, greatly reducing the formation window of the moon.

According to Lars Borg, the lead author of the study: "There were only a few types of materials that could have combined to make the Earth and moon, and they were not exotic — they were likely both just large bodies that formed in approximately the same area that happened to run into one another a little more than 100 million years after the solar system formed… but lucky for us, they did just that."

Putting the pedal to the metal crossing the solid-liquid interface

Most metal alloys are prone to corrosion, which costs hundreds of billions of dollars of damage annually in the U.S. alone. Accurately predicting corrosion rates is a long-standing goal of corrosion science, but these rates depend strongly on the specific operating environment. At the atomic scale, these environmental factors are associated with how quickly and easily metal ions dissolve and transport across solid-liquid interfaces.

Lawrence Livermore National Laboratory (LLNL) scientists have used molecular dynamics simulations to unveil and describe the dynamical behavior of dissolved metal ions and water — a key component of this corrosion puzzle. They introduced a new methodology to describe the strength and nature of chemical bonding between rapidly moving ions in solution. These ions are surrounded by closely held water molecules in the so-called hydration shell, which fluctuates dynamically in ways that can be analyzed computationally. The authors presented a recipe for how these fluctuations could be quantified to ultimately develop computational "descriptors" for the propensity of metals to dissolve in harsh environments. The research appears in in *The Journal of Physical Chemistry Letters.*



Water molecules (shown with red oxygen atoms and white hydrogen atoms) form complex dynamic structures around dissolved metal ions (shown in green). The ease with which these structures can form or break apart often controls the rate at which metals corrode. Image by Stephen Weitzner/LLNL.

Principal Investigator: Brandon Wood

LDRD Project: Predicting and Controlling Corrosion (20-SI-004)

Beyond corrosion, fluctuations in the hydration shell dictate critical processes in interfacial phenomena relevant to a broad array of applications, including water desalination and crystallization, as well as electrochemical energy storage and conversion.

The team came up with three metrics to represent the dynamical softness of ion hydration shells in terms of their rigidity, deformability and fluidity.

"Our analysis showed that the new set of dynamic metrics not only correctly encoded key physical behavior, but also could explain trends in ion behavior that were challenging to classify using conventional static descriptors," said LLNL materials scientist Stephen Weitzner.

Weitzner added that beyond aiding the description and discussion of ion transport kinetics, the metrics provide useful targets for the development of machine learning-based force fields that could dramatically accelerate future simulations of metal ion dissolution and transport rates without loss of accuracy.

LLNL team models COVID-19 disease progression and identifies risk factors

A Lawrence Livermore National Laboratory (LLNL) team has developed a comprehensive dynamic model of COVID-19 disease progression in hospitalized patients, finding that risk factors for complications from the disease are dependent on the patient's disease state.

Using a machine learning algorithm on a dataset of electronic health records (EHRs) from more than 1,300 hospitalized COVID-19 patients with ProMedica — the largest health care system in northwestern Ohio and southeastern Michigan — the team classified patients into "moderate" or "severe" states and tracked disease trajectory as patients moved through different risk states during hospitalization.

Accounting for disease severity — in contrast to previous scientific literature examining only static risk factors — the method allowed the team to identify, as the disease progressed, when certain variables such as age and race, and comorbidities including diabetes and hypertension, led to more severe outcomes.

The model allowed the team, which included co-authors from the University of Toledo, to demonstrate for the first time that links between some factors and more adverse outcomes from COVID-19 can depend on the patient's "current" condition. Most significantly, while male patients were found to be more likely than female patients to have serious complications or die from COVID-19, when starting from the "severe" disease state, women were more likely than men to die of the disease. The results were published in the *Journal of the American Medical Informatics Association*.

"It's well known in the community that men are at a higher risk than women for eventual death from COVID, and that's true — but certain counterintuitive behavior emerges once you break up the patient trajectory into disease states," said LLNL principal investigator Priyadip Ray. "From the moderate disease state, men are more likely to transition to a more severe disease state. However, if you are in the severe disease state, surprisingly, women are more likely to die than men. This disease-state perspective has not been shown before and indicates that where you are in your disease also determines your risk factors."

By modeling the entire trajectory of hospitalized COVID-19 patients, the team showed "statistically significant differences" in the relative risk of disease progression, which they concluded should be taken into consideration when performing risk assessment among patients in hospitals.

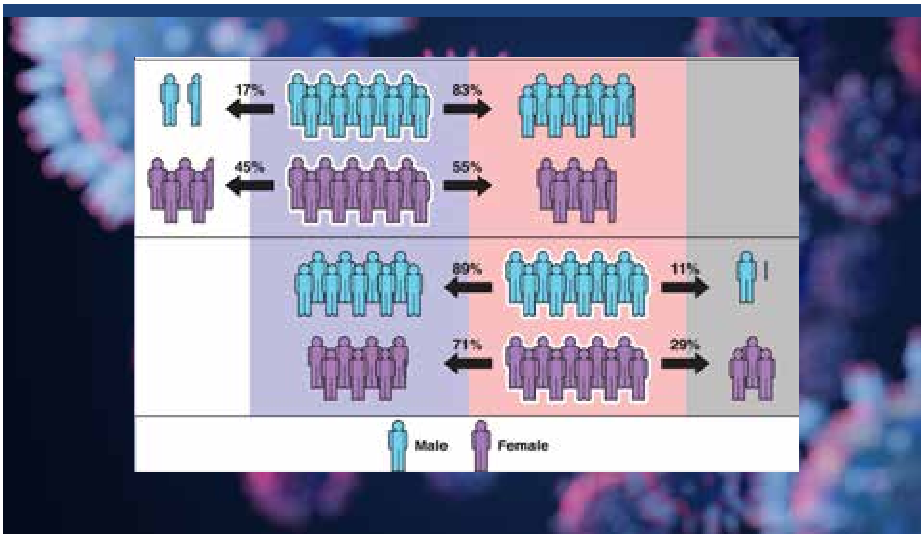
"The vast majority of studies on COVID-19 risk factors ignore the temporal progression of the disease in their analysis," said LLNL co-author Braden Soper. "Our study provides a unique modeling-based approach to understanding how patient demographics and medical comorbidities can present different risk profiles depending on the underlying disease state. Such information is potentially more actionable throughout the course of care, possibly leading to better patient outcomes."

Soper added that disease state-dependent risk assessment also can apply to many other acute and chronic diseases beyond COVID-19, which have thus far largely been assessed only with static data and modeling techniques.

Since EHRs typically suffer from irregularly sampled and/or missing data, the team used a statistical model known as a covariate-dependent, continuous-time hidden Markov model (HMM), known to handle such data well.

The models showed that, while being male, Black, or having a medical comorbidity were all associated with an increased risk of progressing from moderate to severe disease states, the same factors resulted in a decreased risk of transitioning from a severe state to death. Researchers attributed the counterintuitive results to the existing prevalence of static models for risk stratification.

"A fixed-time (static) model is susceptible to immortal time bias, as periods of follow-up may be incorrectly assigned to a particular disease state," Ray said. "An HMM is less susceptible to such biases, as it can infer the disease state throughout the patient trajectory."



Being male is a known risk factor for adverse outcomes in hospitalized COVID-19 patients. However, new analysis reveals that when modeling the entire disease trajectory, the degree to which being male is a risk factor depends on the underlying disease severity of the patient. Foreground image credit: LLNL Principal Investigator Priyadip Ray; Background image credit: Adobe Stock images.

Principal Investigator: Priyadip Ray

LDRD Project: A Deep Bayesian Active Learning Framework for Temporal Multimodal Data (19-ERD-009)

Among the other findings: body mass index (BMI) alone was not linked to an increased risk of disease progression, while old age was associated with an increased risk in progressing from moderate to severe and from severe to deceased states, the researchers reported.

TESTS ON A BUDGET

The LLNL/University of Toledo/ProMedica team's work on dynamic models follows an earlier paper the team published in Scientific Reports, where they examined static risk factors for patients who go on to develop severe complications after testing positive for COVID-19.

The team used an interpretability tool to find out which lab tests were most predictive for hospitalization or poor outcomes, identifying which tests should be collected in the case of budget constraints that could give clinicians nearly the same predictions for adverse outcomes as collecting all possible data.

"We tried to look at this problem in a different way," Ray said. "We asked, 'what if you have a budget constraint? What are the biomarkers that you can collect that will give you a good indication of how likely it is that this patient will need to be ventilated or likely to die due to the disease?' "The interesting thing is that beyond a certain point, collecting more labs will not necessarily give better predictive performance. Can you select a small set of labs and markers that is indicative of risk?" Ray continued. "The answer we found was yes."

To make that determination, the team created a cost structure, grouping types of lab tests and biomarkers with associated costs, from free information (demographics and comorbidities) and low-cost tests such as blood pressure and pulse oximetry, to more expensive lab results — such as liver function and inflammation.

The team then used a machine learning method known to work well for healthcare datasets with missing and/or skewed data to find correlations between patient's features and their risks for death or ventilation from COVID-19 and determine the most predictive set of features. Using the method, they found it was possible to achieve a 43 percent reduction in lab costs with only a 3 percent reduction in performance in predicting the likely need for ventilation from the disease.

Climate change in the Sierra Nevada has profoundly altered its lake ecosystems

Climate change has significantly impacted the natural systems of the Sierra Nevada, including the mountain lakes that are an iconic part of California's natural beauty.

New research from a Lawrence Livermore National Laboratory (LLNL) scientist and colleagues from the University of Kentucky (UK) and Indiana State University (ISU) shows that lake-sediment cores from a subalpine lake in the eastern Sierra Nevada record significant, sometimes abrupt, changes to lake conditions and ecology over the last three millennia.

The Sierra Nevada snowpack serves as the most important water source in the state. Under historical conditions, snow falls on the mountains in the winter and remains frozen until spring. During late spring and summer, meltwater from the snowpack flows into the mountain lakes and streams, ultimately feeding into the major rivers that flow into central and southern California, sustaining vast agricultural fields and urban areas.

Principal Investigator: Ivana Cvijanovic

LDRD Project: Integrating Climate Simulations and Paleontology Data to Constrain California Drought Risks (17-ERD-052)

June Lake beach in the Sierra Nevada of California. Climate change is disrupting the water cycle in the Sierra Nevada in ways that are challenging to predict, which lowers society's resilience by limiting water resources. By studying the changes in fossil diatoms and dating the sediments, the team was able to learn about the aquatic ecosystem's response to climate change.

However, the new study reveals just how dramatically climate change has already impacted aquatic ecosystems in the Sierra Nevada and shows the need for action to protect them. The research appears in the journal *Global Change Biology*.

Anthropogenic climate change is a major factor in recent wildfire activity in California: in 2020, more than 4 million acres of California burned in wildfires, while CalFire reports that more than 2 million acres have already burned in 2021.

The team, which includes LLNL scientist Susan Zimmerman of the Center for Accelerator Mass Spectrometry (CAMS), conducted their study at June Lake, a small subalpine lake in Mono County on the eastern side of the Sierras, popular for fishing and recreation. The team obtained sediment cores from the bottom of the lake and were able to "read" the history of the lake basin recorded in the sediment layers. They used LLNL's signature radiocarbon-dating capability at CAMS, along with the 210Pb method for recent sediments, to determine the age of the various layers.

Historical weather records don't extend far enough back in time to fully understand California's natural climate system, but the lake-sediment records allowed the team to reconstruct the region's climate history over the past 3,000 years. To do this, they studied diatoms, a type of algae that leave behind tiny silica fossils that are preserved in lake sediments. By studying the changes in which types of diatoms dominated the ecosystem in the past, the team was able to learn about the aquatic ecosystem's response to climate change in the Sierra Nevada and when those changes occurred.

The diatoms revealed a detailed history of the lake and its response to changing seasonality, including in the Late Holocene Dry Period and the Medieval Climate Anomaly, which are well-known periods of ancient drought in the region.

But the most striking feature of the fossil record was the uniqueness of the ~1840–2016 period. The team detected the most dramatic changes to the June Lake ecosystem at that time, with the fossils suggesting low water levels, low nutrient concentrations and strong water column stratification. The data suggest that "hot droughts" of the Industrial Era altered the lake state to conditions unseen in the last three millennia and showed that changes attributable to anthropogenic climate change began as early as the mid-19th century.

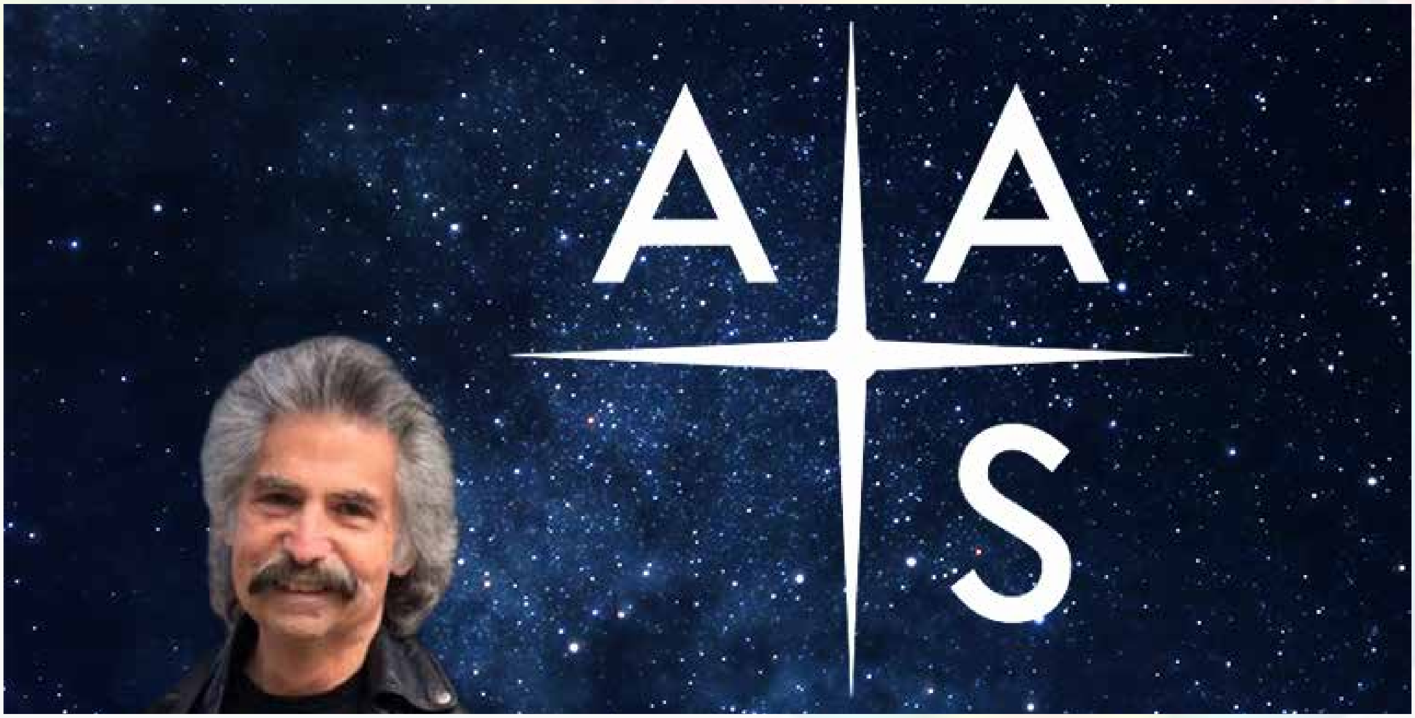
"These results really show the importance of putting climate observations made over the historical period into a longer context." Zimmerman said. "Although California's climate naturally fluctuates between droughts and floods, the conditions we're experiencing now are much more dramatic than even the most severe droughts of the last few thousand years."

"June Lake is a clear example of how sensitive lakes in the Sierras can be to changing climate," said Jeffery Stone, co-author, and professor at Indiana State University (ISU). "Sediment archives like these are one of the few tools we have for recording long-term natural variability and without them we would not be able to clearly observe the profound nature of changes in the lake ecosystem in response to a warming climate."

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 2022, attesting to the exceptional talents of these researchers and underscoring the vitality of Livermore's LDRD program.

FELLOWS



RICHARD KLEIN

Fellow, American Astronomical Society

LLNL physicist Richard Klein was selected for broad and influential contributions to computational astrophysics, for scientific achievements on radiatively-driven stellar winds and star formation theory and for training a generation of students and postdoctoral scholars.

"I am thrilled to get this award designation as a new fellow from the American Astronomical Society. I am deeply grateful to the many extraordinary collaborators, including senior researchers, my graduate students, and postdocs who I have worked with over the last several years both at LLNL and UC Berkeley."

OTHER AWARDS

Sofia Quaglioni and Jennifer Pett-Ridge have been honored as E.O. Lawrence award recipients.

Two Lawrence Livermore National Laboratory (LLNL) scientists are recipients of the prestigious 2021 E.O. Lawrence Award that recognizes mid-career U.S. scientists and engineers for exceptional scientific, technical and engineering achievements related to the broad missions of the Department of Energy (DOE) and its programs.

Jennifer Pett-Ridge was recognized for her research in biological and environmental sciences for pioneering work in quantitative microbial ecology and leadership in developing and applying isotopic tools that help us discover and quantify how changing climate shapes the roles of microorganisms and plants in environmental biogeochemical cycles.

"It feels really wonderful, and both humbling and validating to receive this award," Pett-Ridge said. "I've spent most of my career working with, building up and leading research teams, and our research output speaks to what that collaborative, interdisciplinary approach can enable. I'm not a person with a singular breakthrough — instead I've worked on multiple systems, developed methods, and gained a rich appreciation for both fundamental and applied questions. It means so much to me that DOE and the review committee valued that kind of career path."

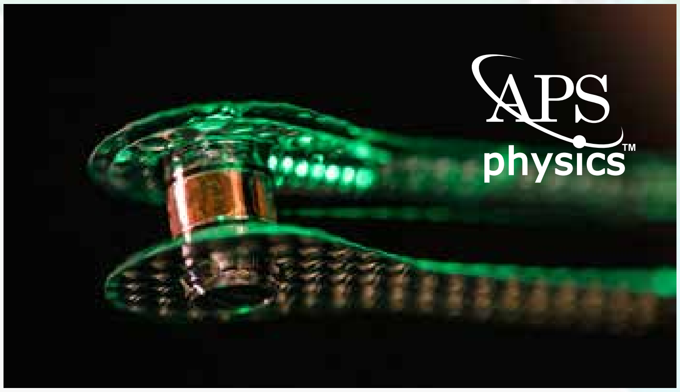
Sofia Quaglioni was cited for her work in nuclear physics, specifically for seminal contributions unifying the theory of structure and reactions of light nuclei, providing predictive capability critical for understanding inertial fusion and nuclear astrophysics, as well as pioneering applications of quantum device simulations for nuclear dynamics.

"I am thankful to the DOE Office of Nuclear Physics for funding my research for the past 15 years, and to all the friends and colleagues who have supported and encouraged me," Quaglioni said. "Most of all, I am thankful to my loving husband and two wonderful boys for their infinite patience and for always believing in me."

The Lawrence Award was established to honor the memory of Ernest Orlando Lawrence, who invented the cyclotron — an accelerator of subatomic particles — and was named the 1939 Nobel Laureate in physics for that achievement. Lawrence later played a leading role in establishing the U.S. system of national laboratories, and today, the DOE's national laboratories in Berkeley and Livermore bear his name.

OTHER AWARDS

Burning Plasma Team receives honor from American Physical Society



The Burning Plasma Team has been awarded the 2022 John Dawson Award for Excellence in Plasma Physics Research by the American Physical Society. The team consists of members from Lawrence Livermore National Laboratory (LLNL) and from other institutions.

The team was cited "for the first laboratory demonstration of a burning deuterium-tritium plasma where alpha heating dominates the plasma energetics."

"This honor recognizes the hard work and dedication conducted by the Burning Plasma Team in achieving and entering the burning plasma regime in a laboratory," said Mark Herrmann, director for the Weapon Physics and Design Program within LLNL's Weapons and Complex Integration Directorate."

Richard Kraus honored for inaugural American Physical Society award

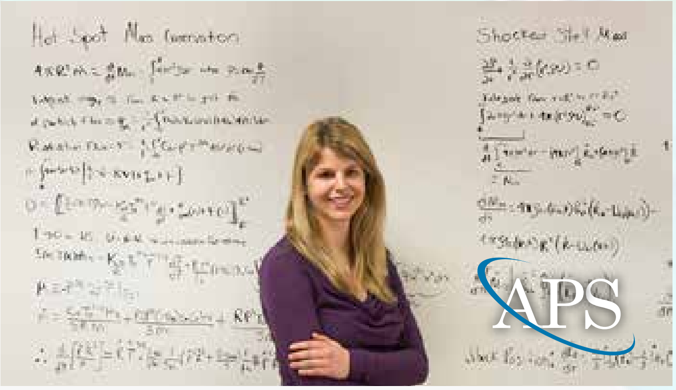
Lawrence Livermore National Laboratory (LLNL) research scientist Richard Kraus is the recipient of the inaugural American Physical Society's 2023 Neil Ashcroft Early Career Award for Studies of Matter at Extreme High Pressure Conditions. Kraus is recognized for his outstanding theoretical or experimental contributions by an early-career scientist to studies of matter at extreme high-pressure conditions.

"To receive the inaugural Neil Ashcroft award is such an incredible honor. I hope that I can continue some of Neil's legacy, pushing at the frontiers of our field while improving my ability to communicate the importance of what we do to a broader audience and the next generation of early-career scientists."

Kraus received his Ph.D. in earth and planetary sciences and master's in applied physics from Harvard University, and master's and bachelor's degrees in physics from the University of Cambridge and the University of Reno, respectively.

OTHER AWARDS

Lab scientist wins outstanding doctoral thesis award from American Physical Society



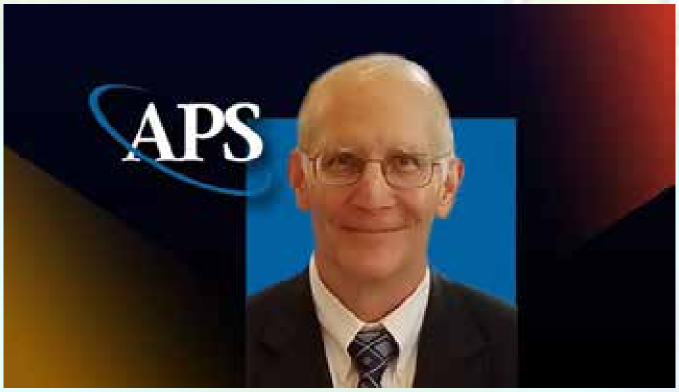
Lawrence Livermore National Laboratory (LLNL) scientist Alison Ruth Christopherson has earned the American Physical Society's (APS) Marshall N. Rosenbluth Outstanding Doctoral Thesis award.

The award recognizes exceptional early-career scientists who have performed original thesis work of outstanding scientific quality and achievement in the area of plasma physics.

Christopherson was honored "for theories of fusion alpha heating and metrics to assess proximity to thermonuclear ignition in inertially confined plasmas, and for the development of a novel measurement of hot electron preheat and its spatial distribution in direct-drive laser fusion."

"It is an honor to receive an award named after the extraordinary scientist Marshall Rosenbluth, whose brilliance laid the foundations for multiple fields within plasma physics," Christopherson said. "He set the bar impossibly high for the rest of us."

Bruce Remington honored with American Physical Society award



Bruce Remington, a distinguished member of the technical staff at Lawrence Livermore National Laboratory (LLNL), has been honored with the American Physical Society's (APS) 2023 George E. Duvall Shock Compression Science Award, which recognizes contributions to understanding condensed matter and non-linear physics through shock compression. Remington was specifically honored "for pioneering laser-driven high-pressure, solid-state material dynamics in high-energy density regimes."

"This award suggests to me that our high-energy-density science (HEDS) focus area has matured to the level that it is accepted and now highlighted for recognition by the broader shock physics community. This is a rewarding milestone for our HEDS community," Remington said.

Remington received his bachelor's degree from Northern Michigan University in 1975 and his Ph.D. in nuclear physics from Michigan State University in 1986. He did a two-year postdoctoral appointment in nuclear physics at LLNL, then joined the Laser Program (now the National Ignition Facility [NIF] and Photon Science Directorate) at LLNL in 1988. Since 1988, he has been a staff physicist in the Inertial Confinement Fusion (ICF) Program followed by the High Energy Density Science Program. He has been the NIF Discovery Science Program leader since 2014. He is best known for his work in HED laboratory astrophysics, where he founded the High Energy Density Laboratory Astrophysics conference series in 1996 to foster this new science focus area.

OTHER AWARDS

LLNL physicist Debbie Callahan receives fusion leadership award

The Fusion Power Associates (FPA) Board of Directors has selected Lawrence Livermore National Laboratory (LLNL) physicist Debbie Callahan as a recipient of its 2022 Leadership Award.

Callahan received the award at the Fusion Power Associates 43rd Annual Meeting and Symposium, in Washington, D.C. FPA leadership awards have been given annually since 1980 to recognize persons who have shown outstanding leadership qualities in accelerating the development of fusion as a commercial power source.

“I'm honored to have been selected for this award and be in the company of other great leaders in fusion — both at LLNL and around the world,” Callahan said. “I've spent my career in fusion — first in inertial fusion energy and then moving to working towards ignition on NIF. It's been an incredible journey of interesting science and technology and I've gotten to work with a great team of people in ICF and NIF.”

Callahan joined LLNL in 1987 as a graduate student in the Department of Applied Science, UC Davis. She received her Ph.D. in 1993 and was hired into X Division as a postdoc working on inertial fusion energy. She has spent her career working on inertial fusion energy (IFE) and inertial confinement fusion (ICF). She has authored or co-authored more than 200 refereed journal publications.

LLNL researchers win HPCwire award for applying cognitive simulation to inertial confinement fusion

The high performance computing publication HPCwire announced Lawrence Livermore National Laboratory (LLNL) as the winner of its Editor's Choice award for Best Use of HPC in Energy for applying cognitive simulation (CogSim) methods to inertial confinement fusion (ICF) research.

Members of the CogSim team include LLNL researchers Brian Spears, Timo Bremer, Luc Peterson, Kelli Humbird, Rushil Anirudh, Brian Van Essen.

The award recognizes the team for progress in their machine learning-based approach to modeling ICF experiments performed at the National Ignition Facility (NIF) and elsewhere, which has led to the creation of faster and more accurate models of ICF implosions.

Spears said. “I'm particularly grateful to the wonderful team that we have used to build the tools and techniques over the years. What's most exciting to me and the rest of the team is that we've worked very hard to build AI into a tool that can bridge high-performance computing and experimental work and put that together into something that's actually functional for science.

“It's really a large thrust from many different projects all working together — energy, fusion, CogSim — so it's really awesome to see people from physics to computer science workflows all working together to get this done,” Bremer said. “And then to have this recognized is really a great honor.”

Added Van Essen: “The ability to work with this multidisciplinary team to develop these novel models and methods for scaling the training of deep neural networks for strategically important science is an absolute blast and a highlight of working at the national laboratories.”

OTHER AWARDS

2022 Gulbenkian Prize for Humanity jointly awarded to the IPCC

The United Nations (UN) Intergovernmental Panel on Climate Change (IPCC) was jointly awarded the Gulbenkian Prize for Humanity, alongside the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES). The prize jury distinguished the two intergovernmental organizations for their role in developing scientific knowledge, alerting society, and informing policymakers to improve decision-making to combat the dual challenges of climate change and biodiversity loss.

LLNL climate scientists have contributed as invited authors to every one of the six IPCC Assessment Reports since the first (FAR) was released in 1990 through to the latest Sixth Assessment Report (AR6), released in August 2021, and shared the Nobel Peace Prize with Al Gore in 2007 for these roles. The reports have documented and anchored global climate knowledge, melding the latest in observation and climate-model-based science.

The Gulbenkian Prize for Humanity was launched by the Calouste Gulbenkian Foundation in 2020 with the objective of distinguishing those persons and global organizations whose work has greatly contributed to mitigating the impacts of climate change.

Two LLNL-led papers win Test of Time awards at 2022 IEEE VIS conference

Two Lawrence Livermore National Laboratory-led teams received SciVis Test of Time awards at the 2022 IEEE VIS conference for papers that have achieved lasting relevancy in the field of scientific visualization.

Published in 2008, an LLNL-led paper that — for the first time — allowed Digital Morse Theory to be applied to large scale and three-dimensional data, won the 14-year Test of Time award for making a lasting impact to the decades-long application of computational topology to data analysis and visualization at scale. LLNL co-authors included at the time were LLNL graduate research student Attila Gyulassy and computer scientists Peer-Timo Bremer and Valerio Pascucci.

LLNL's Bremer said the paper was the culmination of work that began with "a fundamental mathematical theory and ended in eminently practical and scalable algorithms."

The SciVis 25-year Test of Time award went to a paper co-authored by former LLNL senior scientist Mark Duchaineau and current LLNL computer scientist Mark Miller, who has helped develop numerous scientific database, visualization, and data modeling technologies at LLNL.

"Most of the ideas lived on," Duchaineau said. "My colleagues and I were delighted to see how these ideas spread and were extended and adapted in so many ways."

OTHER AWARDS

DOE Office of Science Early Career Research Program Award

DOE honors three early-career Lab scientists

Three scientists from Lawrence Livermore National Laboratory (LLNL) are recipients of the Department of Energy's (DOE) Office of Science Early Career Research Program award.

Mimi Yung, John Despotopulos and Timofey Frolov are among 83 awardees receiving the recognition. Under the program, typical awards for DOE national laboratory staff are $500,000 per year for five years.

Yung, a biochemist, was selected for her work in biological and environmental research, Despotopulos was selected for his research in nuclear physics, and Frolov was chosen for his work in fusion energy sciences.

"I feel incredibly grateful and truly honored to receive this award. It is a real highlight of my career thus far," Yung said.

John Despotopulos was nominated for his work in the measurement of neutron-induced cross sections of nuclides, that has implications for national security and can improve our understanding of stellar nucleosynthesis.

"I'm shocked at receiving the award and excited to be able to perform this research," he said.

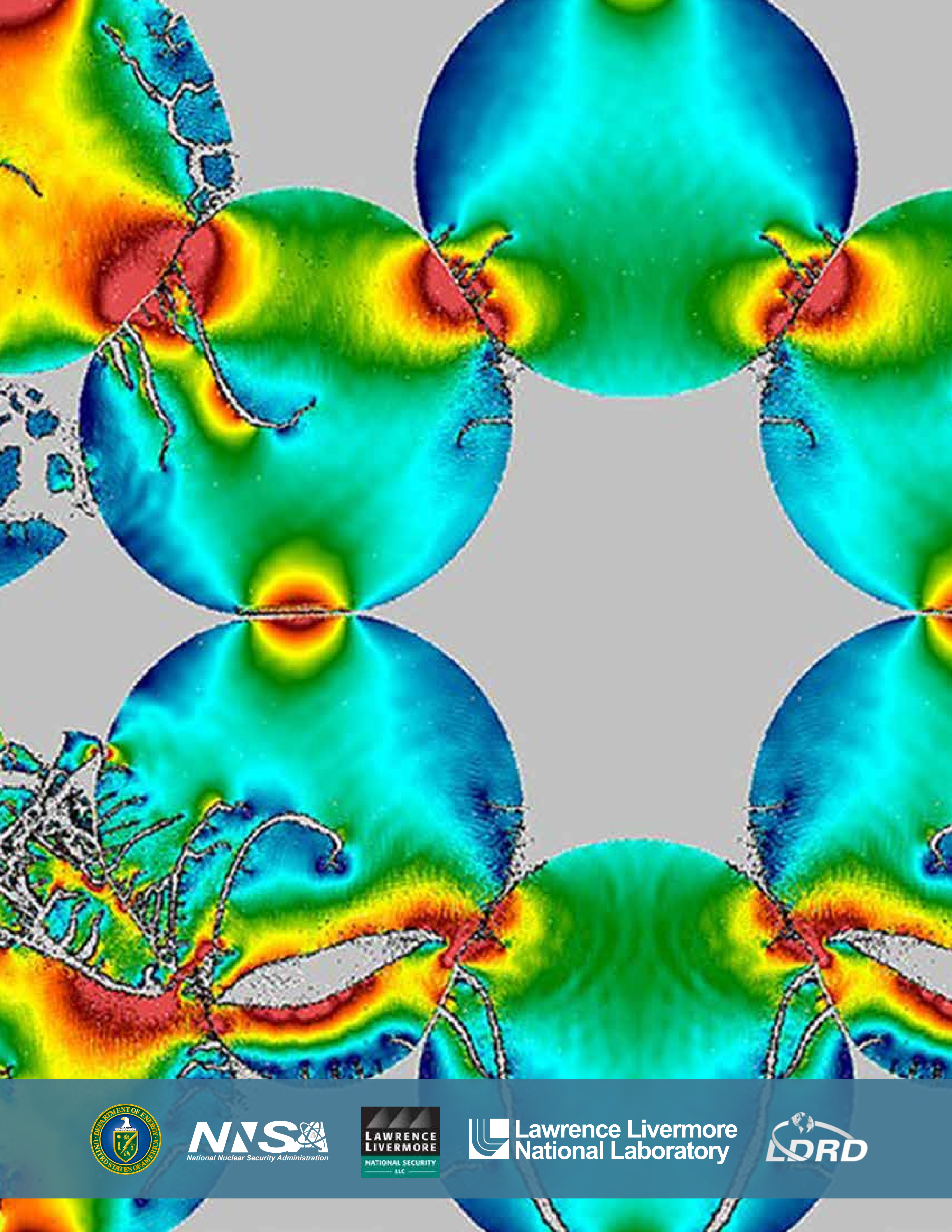
Timothy Frolov is a physicist in the Materials Science Division and was nominated in the fusion energy sciences division for his work in grain boundary structure engineering of resilient tungsten alloys for fusion applications.

"I am excited about receiving this award and continuing my research," Frolov said.

"Supporting America's scientists and researchers early in their careers will ensure the U.S. remains at the forefront of scientific discovery and develops the solutions to our most pressing challenges," said U.S. Secretary of Energy Jennifer M. Granholm. "The funding will allow the recipients the freedom to find the answers to some of the most complex questions as they establish themselves as experts in their fields."

The Early Career Research Program, now in its 13th year, is designed to bolster the nation's scientific workforce by providing support to exceptional researchers during crucial early-career years, when many scientists do their most formative work.

Cover image: Numerical simulation of dynamic fracture, comminution, and compaction of a brittle granular material. Color contours show shear stress with black indicating damaged material and fracture surfaces. Simulations performed by Michael Homel using the LLNL GEOS Material Point Method (MPM) code, which provides robust tools for modeling large-deformation, contact, and fracture of brittle materials as described in: Homel, Michael A., and Eric B. Herbold. "Field-gradient partitioning for fracture and frictional contact in the material point method." International Journal for Numerical Methods in Engineering 109.7 (2017): 1013-1044.



NNSA National Nuclear Security Administration

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Lawrence Livermore National Laboratory

LDRD