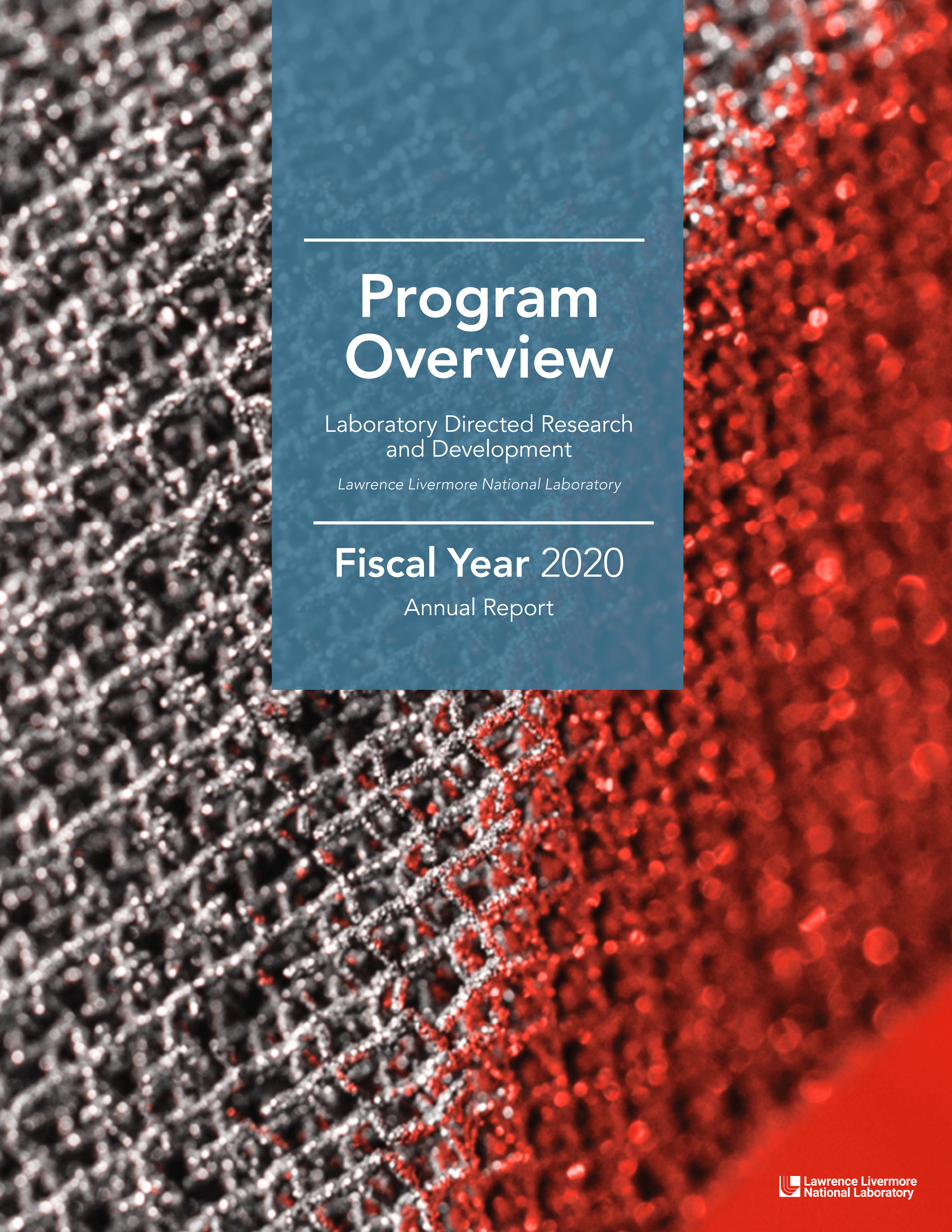

Program Overview

Laboratory Directed Research and Development

Lawrence Livermore National Laboratory

Fiscal Year 2020

Annual Report

Lawrence Livermore National Laboratory

Annual Program Overview

Over the last three decades, the Laboratory Directed Research and Development (LDRD) Program has enabled Lawrence Livermore to fund research that addresses the national security challenges we face today, as well as future mission needs. In this annual report, we provide an overview of how these targeted investments allow LLNL to develop cutting-edge capabilities and foster innovation in key programmatic areas.

One noteworthy example that I am especially proud of is how LDRD investments allowed us to help our nation quickly respond to the COVID-19 pandemic, funding 5 projects during the first few months of the pandemic. These projects illustrate how the LDRD program advances our Lab's mission agility.

In this report, we describe how investigators leveraged our capabilities in bioscience, data science, and high-performance computing to accelerate solutions in multiple areas, including new diagnostic capabilities, therapeutics, and other types of medical countermeasures to combat the virus.

In addition, LDRD investments focus on fostering the technical vitality needed to fulfill our mission. For example, investigators are exploring new ways to address challenges in nuclear weapons science, nuclear threat reduction, space security, cybersecurity, and energy security. As you browse this report, you will learn about projects that utilize LLNL's core competencies in areas such as advanced manufacturing, optics, high-performance computing, and simulation.

Finally, our LDRD program makes it possible for us to cultivate the creativity of the Lab's most important resource—our workforce. LDRD-sponsored research enables us to expand our outreach to tomorrow's innovators, as we mentor students and onboard postdoctoral researchers, while developing the leadership capabilities of early career staff. The mentorship aspect of our program is one of its hallmarks. A multidisciplinary group of senior scientists and other advisors encourage our staff to pursue new research directions.

Throughout this year's report, we highlight how the LDRD program invests in ideas that make the world a safer place. We review key accomplishments and performance indicators, and we share snapshots of some of our talented staff. I also encourage you to visit our LDRD website and learn more about the 244 projects that we supported during fiscal year 2020. Looking to the future, I am confident that LDRD investments will continue to help LLNL remain at the forefront of innovative research.

William H. Goldstein
LLNL Director

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

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.

Program Oversight

Day-to-day oversight of our program is provided by LDRD Program Director Doug Rotman. However, 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 programmatic leaders. This local team works closely with NNSA's Livermore field office, NNSA's LDRD program leaders, and LDRD program leaders at the Department of Energy.

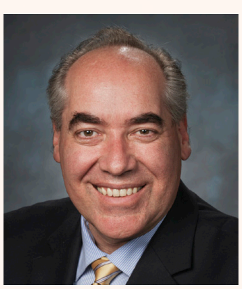
At the programmatic level, LDRD portfolio management at Livermore is structured to assure alignment with DOE, NNSA, and Laboratory missions. Designated LDRD points of contact for each of the Laboratory's strategic investment areas provide input regarding LDRD investment priorities to Livermore's senior 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, these programmatic 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 Indicators Drive Program Improvement

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.

In FY20, the working group finalized a combination of common quantitative and qualitative long-term indicators, emphasizing a systematic approach to tracking and reporting performance indicators. For the first time, as each institution issues its LDRD program report for fiscal year 2020, we are presenting a common set of long-term performance indicators, which can be found in the Program Value section of this report. Our report also includes performance indicators specified by DOE's director of LDRD programs, in accordance with DOE Order 413.2C.



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

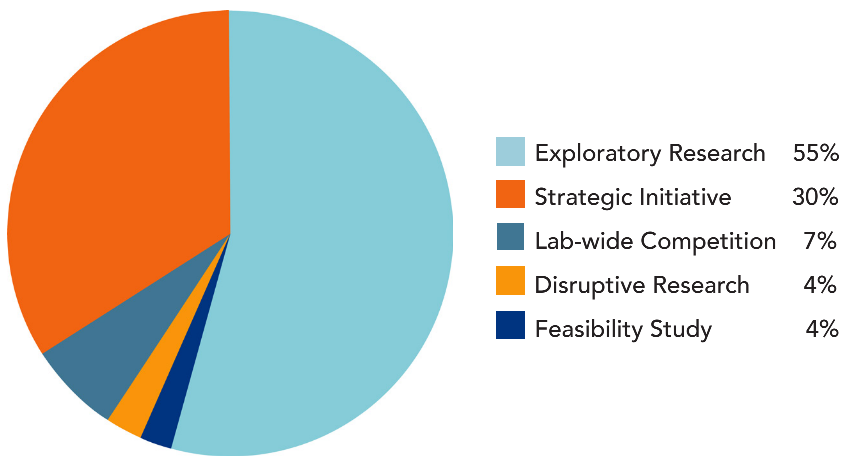
LDRD investments span a broad range of research topics, helping to ensure that LLNL supports innovation in key programmatic areas. Funded projects address some of our newest mission spaces, including cognitive simulation, predictive biology, space science and security, and hypersonic science. We also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

For fiscal year 2020, 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 FY20 investment portfolio reflect this structure, including how funds are distributed across the program's 5 types of projects and 17 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.

FY20 INVESTMENTS
244 PROJECTS
$121M TOTAL FUNDING

Funding by Project Type

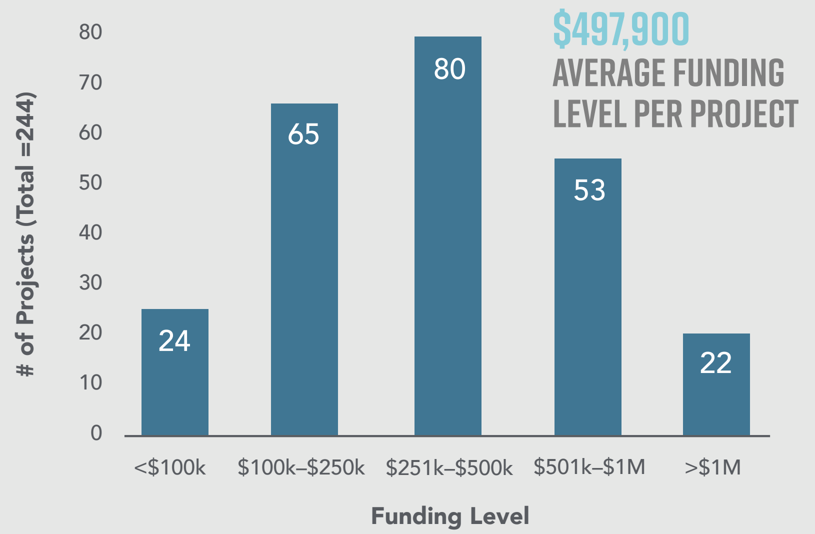
Livermore's LDRD program includes five types of projects. Each one has a distinctive purpose, duration, and funding limits. For example, our one-year feasibility studies support relatively brief investigations of a specific technical approach. These types of projects can be launched mid-year to rapidly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



Project Type	FY20 Projects Funded	Project Aim
Exploratory Research	139	Address a specific research challenge or enhance a core competency.
Feasibility Study	49	Determine the viability of a new way to address a mission-relevant challenge.
Lab-wide Competition	32	Conduct innovative basic research and enable out-of-the-box thinking.
Strategic Initiative	15	Make significant progress addressing a mission-relevant challenge from a multidisciplinary perspective.
Disruptive Research	9	Pursue novel ideas with the potential to overturn fundamental paradigms or create new research directions.

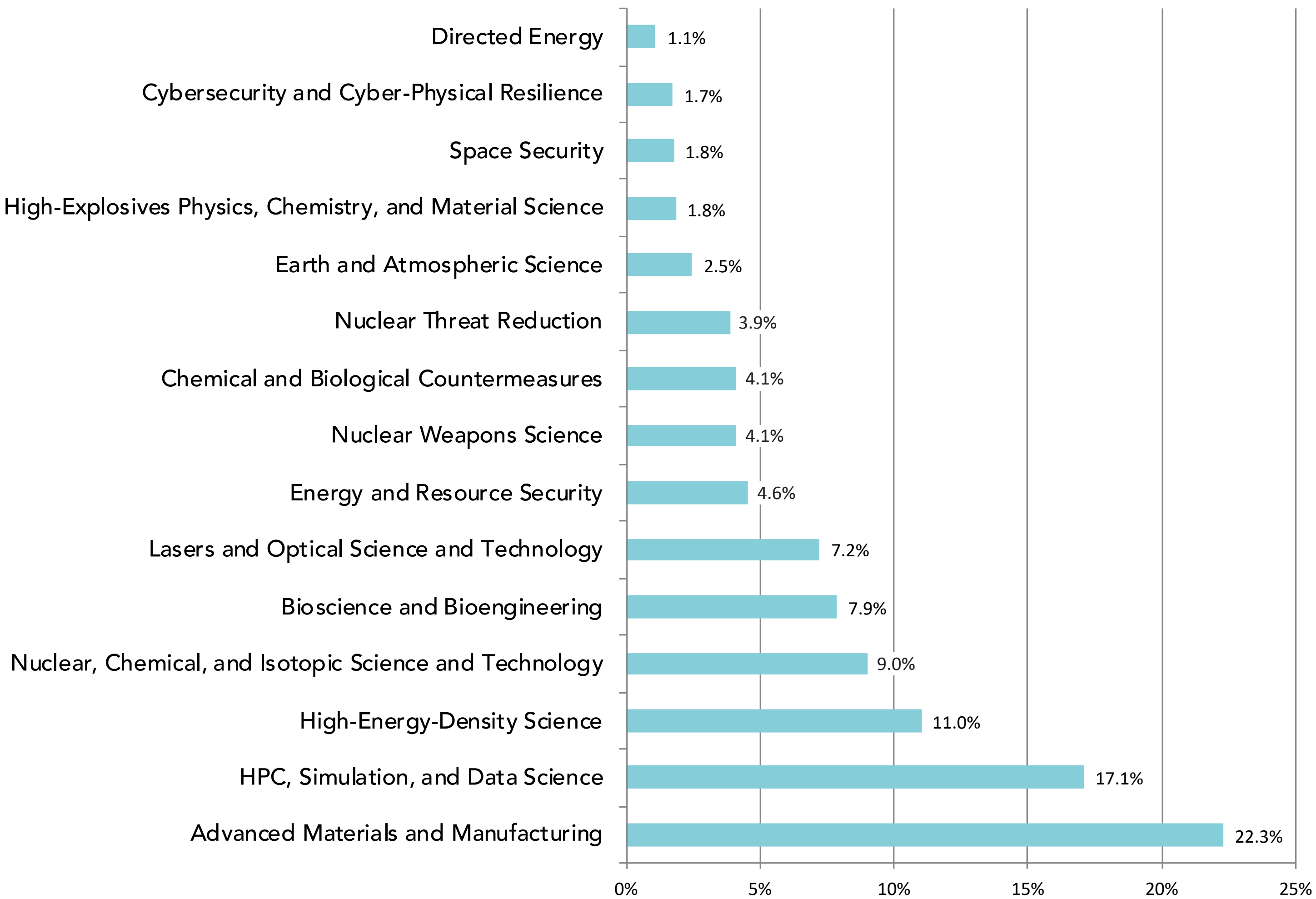
Projects by Funding Level

Our Laboratory's investment strategy includes the flexibility to fund projects at varying dollar amounts, depending on the project scope. This chart presents data on the number of projects funded in FY20, distributed across five funding levels. The largest number of projects (80) fell in the middle funding range, receiving between $251k and $500k per project. A smaller number of projects received less than $100k in funding (24 projects), or more than $1M in funding (22 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 10 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. For FY20, Forensic Science was only listed as a secondary research focus.)



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

56 INSTITUTIONS were involved in formal collaborations with LLNL as part of LDRD-funded research teams in FY20.

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	FY16	FY17	FY18	FY19	FY20
LDRD-funded projects with one or more formal collaborations	45	62	74	74	78
Percentage of all projects at LLNL	25%	29%	31%	30%	32%

Innovative design of 3D-printed electrodes increases catalytic activity

Rechargeable metal–air batteries show tremendous promise for safe, low-cost, high-capacity energy storage, offering an alternative to lithium–ion batteries that are reaching their energy density limit. However, the energy-delivery capacity of metal–air batteries is currently constrained by sluggish kinetics that limit the catalytic activity of these compact power sources.

An LDRD-funded research team at LLNL partnered with investigators from two University of California campuses—Santa Cruz and Merced—to improve the catalytic potential of metal–air batteries. They developed a new electrode design that rapidly eliminates the gas bubbles that can get trapped in the material and reduce current density.

“The gas bubbles that are created during electrolysis often mingle together and get trapped,” explained the project’s lead investigator, LLNL materials scientist Cheng Zhu. “Our new electrode design pulls out the bubbles as quickly as possible so they don’t reduce the electrode’s catalytic activity.”

While developing the electrode’s architecture, the team used simulations to explore how the gas bubbles form, how they escape, and the rate at which they escape. The structural modeling enabled the team to explore the physics going on inside the electrodes and identify ways to more effectively manage bubble migration through a hierarchical porous structure.

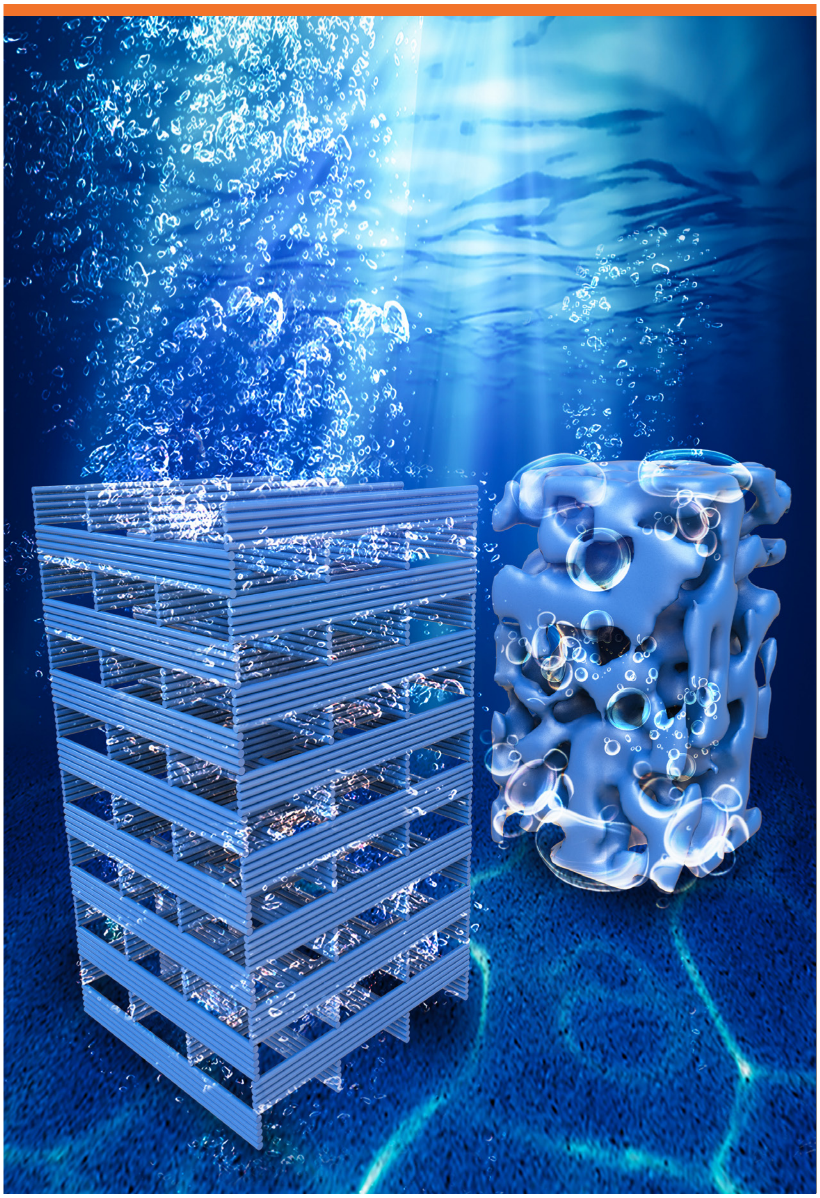


Illustration depicting the novel 3D electrode design that manages gas-bubble migration—developed by LLNL researchers, in collaboration with investigators from two University of California campuses.

The team designed, fabricated, tested, and optimized the structure of the three-dimensional (3D) printed electrode, demonstrating that it can eliminate the physical barrier between catalyst and reactant, and significantly improve the electrode’s current density.

“While other investigators have studied the material side of electrolysis, this team showed that the actual architecture of the components matter just as much as the materials, especially at high production rates,” said Brandon Wood, who leads LLNL’s research initiatives in hydrogen energy materials.

By improving the catalytic activity of advanced batteries, this research provides a promising pathway to further enhance energy storage capabilities, as well as our nation’s ability to deliver clean, hydrogen-based energy.

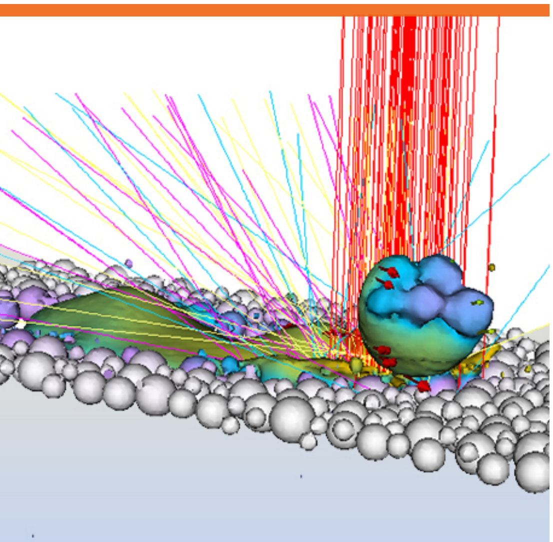
Principal Investigator: Cheng Zhu

LDRD Project: Rational Design of Bifunctional Electrocatalysts for Rechargeable Metal–Air Batteries

Principal Investigator: Ibo Matthews

LDRD Project: A New Science-Based Paradigm Enabling Microstructure-Tailored Additive Manufacturing of Metals

Simulations identify novel way to mitigate defects and customize laser-driven metal fabrication



An illustration of the simulation used by the research team, which included collaborators from the Air Force Research Laboratory. The illustration depicts a laser interacting simultaneously with the melt pool and a large spatter of metal powder particles. In this event, the laser's power was above a threshold that expelled the spatter away from the scan track. This approach prevented formation of defects due to laser shadowing, in which melted metal powder can block or eclipse the laser.

In collaboration with investigators at the Air Force Research Laboratory, LLNL scientists tackled a challenge associated with laser-based metal fabrication, tapping into multi-physics simulation capabilities to identify a novel solution. Experiments alone could not fully explain the dynamics behind a process that causes defects when using a laser-based additive manufacturing (AM) process to form 3D metal parts.

When fabricating 3D parts using laser powder-bed fusion, where a laser beam melts metal powder layer-by-layer to form parts, clusters of powder particles ejected from the laser's path can land back on the parts and potentially lead to defects. During this LDRD-funded research project, investigators explored the mechanisms behind how this "spatter" forms, and how to modify the fabrication process to prevent large amounts of spatter.

Since experiments lack the required spatial and temporal resolution to follow the fast dynamics (approximately 1 microsecond) behind the laser-spatter interactions, researchers used computer models to create a digital twin of the process. Using the predictive model, along with high-speed x-ray and optical imaging, they established a stability criterion, creating a power map that controls the laser's power output along its scan vector, thereby maintaining a stable melt pool and avoiding large amounts of spatter.

According to Ibo Matthews, who led the LDRD project and has analyzed melt-pool dynamics for several years, modulating the laser power makes it possible to avoid disturbing the powder bed. "The ability to control the energy input using validated models opens up pathways to defect mitigation, as well as material enhancement through tailored microstructure engineering," said Matthews.

The team anticipates that the model-driven scanning strategy, which includes precise temporal and spatial control of the laser-energy source, will improve overall part reliability by enabling more uniform properties of 3D-printed parts. In addition, the new approach may also enable opportunities to use this additive manufacturing technique with new types of materials that traditionally fail during a part build.

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-fifth of the Laboratory's copyrights (chiefly computer code), and about half of the Laboratory's records of invention.

Patents	FY16	FY17	FY18	FY19	FY20
All LLNL patents	97	88	79	143	200
LDRD patents	54	55	41	95	131
LDRD patents as a percentage of total	56%	63%	52%	66%	66%

LDRD-funded work has played a key role in developing **MORE THAN 50%** of the Laboratory's patents.

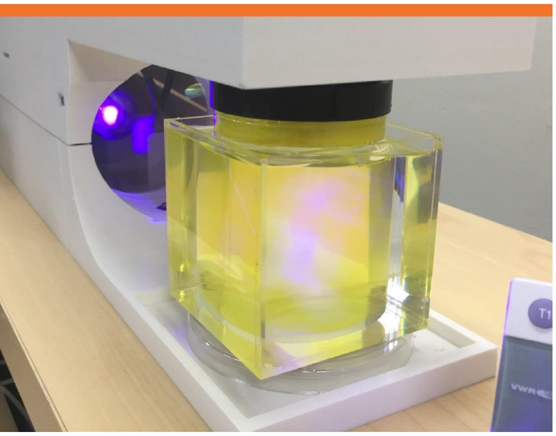
Copyrights	FY16	FY17	FY18	FY19	FY20
All LLNL copyrights	72	105	105	118	138
LDRD copyrights	19	19	23	24	31
LDRD copyrights as a percentage of total	26%	18%	22%	20%	22%

Records of Invention	FY16	FY17	FY18	FY19	FY20
All LLNL records	91	110	105	129	126
LDRD records	43	53	47	65	56
LDRD records as a percentage of total	47%	48%	45%	50%	44%

Principal Investigator: Maxim Shusteff

LDRD Projects: Advanced Photopolymer Materials Engineering for Multiscale Additive Fabrication

Three-Dimensional Fabrication by Tomographic Holographic Lithography



A patented technology developed through LDRD-funded research, known as computed axial lithography, uses photons to project a series of computer-generated images into a container of photosensitive resin while the container slowly rotates. After a few minutes, the fluid is drained, leaving behind a fully-formed 3D object suspended in the resin.

Volumetric additive manufacturing enables fabrication of 3D-printed objects in a single step

A breakthrough technology developed by LLNL investigators in collaboration with researchers at the University of California, Berkeley, creates an entire three-dimensional part at once, rather than in a series of steps. The idea for this innovative approach to additive manufacturing started several years ago, and through a series of LDRD-funded projects, it has now resulted in a patented technology with a broad array of applications—including national security, aerospace, optics, medicine, dentistry, and energy delivery.

In the patented process known as computed axial lithography (CAL), a projector beams a series of computer-generated images into a container of photosensitive, syrup-like resin while the container rotates. After a few minutes, a fully-formed 3D object solidifies, suspended in the resin, and the remaining liquid can be drained. Uniquely shaped polymer parts with complex geometries can be made much more quickly with CAL than with layer-by-layer fabrication methods.

According to Maxim Shusteff, an LLNL engineer who led both LDRD-funded projects, the goal of this research was to develop a technique that could overcome the drawbacks of layer-by-layer 3D printing, where each layer takes a minute to print. With parts that can include hundreds of layers, it can take a long time to print each part. In addition, the resulting parts often have undesirable properties, such as rough edges or disconnected islands of material.

In contrast, this novel volumetric AM approach enables an object to be supported by the buoyancy of the surrounding liquid as it is fabricated. "We can print extremely delicate microstructures in soft materials," said Shusteff. "CAL eliminates many of the fabrication constraints that engineers and the bioprinting community have been facing for a long time."

As industry collaborators explore new applications for this innovative technology, the LDRD-funded research team at LLNL is exploring new types of photocurable materials that can be used with CAL to fabricate a broader range of parts.

"Available polymers present limitations such as brittleness and poor aging performance that can occur months or years after curing is completed," Shusteff explained. "Our current research focuses on developing photocurable materials for AM with architectures that provide superior mechanical properties, along with dependable lifetime performance."

Current industry partners include a bioprinting company and an advanced materials company. Each partner is exploiting different features of the volumetric AM approach to increase the competitive technological edge of their products.

Tailored glass optics offer design flexibility for laser applications

Principal Investigator: Rebecca Dylla-Spears

LDRD Project: Glass Inks for Three-Dimensional Printed Fiber Preforms and Telescope Optics

An innovative optical technology developed through a series of LDRD-funded projects, initially demonstrated for laser applications, may also help address industry needs related to improving lightweight optical systems.

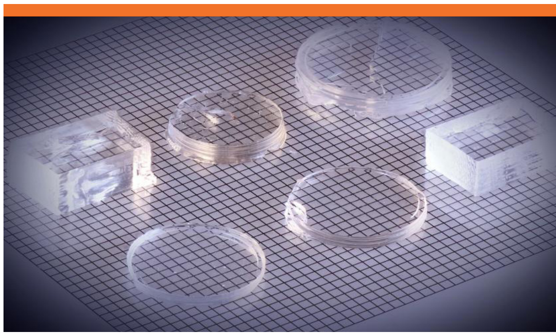
Research started in 2016, when the LDRD team began exploring ways to additively manufacture optics with the physical shapes and refractive-index profiles of interest for reducing the size, weight, and power of optical systems. Because additive manufacturing offers the ability to control both structure and composition, the research team was able to modify what had historically been a highly constrained design process, instead providing the design flexibility needed to produce gradient-refractive-index optics with the desired sizes and profiles.

LLNL investigators focused on the material composition needed to create tailored, lightweight optics, along with innovative approaches to fabricate optical components with unique structures. They used an additive manufacturing technique known as direct-ink writing (DIW), enabling them to actively control the ratio of glass-forming feedstock materials as they were blended together. For example, they used specially formulated silica-containing pastes or resins, and by changing the proportions of the different types of inks while printing, they were able to alter the refractive index. After the optical preform is built, it is densified to glass, and can be finished using conventional optical polishing.

"The change in material composition leads to a change in refractive index once we convert it to glass," explained LLNL chemical engineer Rebecca Dylla-Spears, who leads LLNL's multidisciplinary research team that includes experts in materials science, optical engineering, and laser technology.

The technique is expected to enable scientists to produce lightweight, environmentally stable, flat glass components (with no surface curvature). The gradient-refractive-index optics alter how light travels through the medium, so that the lens can have a flat surface, yet still perform the same optical function as an equivalent conventional lens.

LLNL scientists are exploring potential industry applications of this technique, including the ability to produce lightweight, tailored components for optical systems.

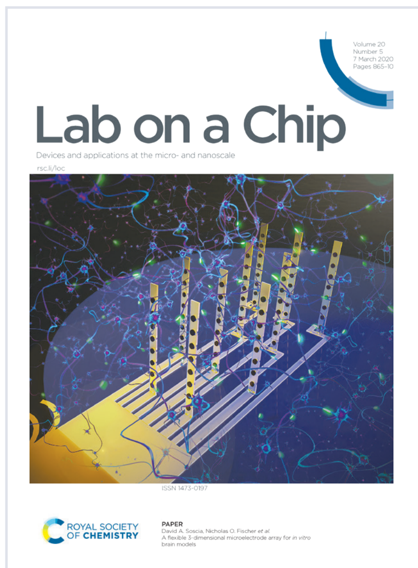


LLNL scientists developed an innovative approach to produce small, robust, lightweight optics in varying shapes, including optical elements that are flat on both sides, yet still perform the same optical function as a conventional lens by varying the material's refractive index (rather than its shape).

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	FY16	FY17	FY18	FY19	FY20
All LLNL articles	1,041	1,126	1,178	1,281	1,149
LDRD articles	265	274	456	553	428
LDRD articles as a percentage of total	25%	24%	39%	43%	37%



LDRD Project: An Investigational Platform of the Human Brain for Understanding Complex Neural Function

Principal Investigator: Nick Fischer

LDRD-funded research regarding modeling the human central nervous system was featured on the cover of the *Lab on a Chip* journal and an article describing how the team developed a thin-film, three-dimensional, flexible, microelectrode array (3DMEA) that non-invasively monitors a 3D culture of neurons and records neuronal function.

The platform is an important step in facilitating non-invasive electro-physiological characterization of 3D networks of electroactive cells in vitro. This capability can enhance our understanding of how the human brain responds to infection, disease, and chemical exposure, underpinning the development of therapies and therapeutics.

Principal Investigator: T. Yong Han

LDRD-funded research was also featured on the cover of the *Journal of Chemical Information and Modeling*, highlighting efforts to leverage the capabilities of machine learning to accelerate materials discovery and optimization. As highlighted in the article, the team developed a machine learning tool that that can extract and structure information from the text and figures in scientific publications regarding nanomaterials.

The research team tapped into their expertise in materials science and data analytics to develop an automated information-extraction pipeline that uses natural-language processing image analysis and visualization techniques to identify and analyze microscopy images of nanomaterials and determine their morphologies and size distributions. They also created a knowledge base regarding nanomaterials synthesis that can be mined to help inform further nanomaterials development.

Since concluding their LDRD-funded project, the research team has applied their machine learning tools to extract information from the SARS-CoV-2 and COVID-19 literature, which is being analyzed for its utility in accelerating COVID-19 research.

LDRD Project: Materials Informatics for Synthesis, Optimization, and Scale-Up of Advanced Materials

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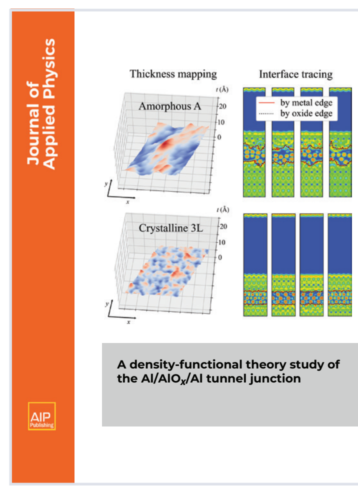
Principal Investigator: Vince Lordi

LDRD-funded research was featured in the *Journal of Applied Physics*. The article was one of many scientific publications produced as part of an LDRD exploratory research project, where investigators developed a new, computationally efficient modeling framework to predict how superconducting circuits respond in the quantum regime.

As highlighted in the article, investigators used first-principles modeling to assess fundamental aspects of the atomic structure of amorphous and crystalline tunnel junctions, which are critical components of superconducting circuits used in quantum computers. The project contributes enabling capabilities to support long-term needs in quantum-coherent superconducting device design for sensors, simulation, and information processing.



LDRD Project: Predictive Modeling of Correlated Noise in Superconducting Circuits

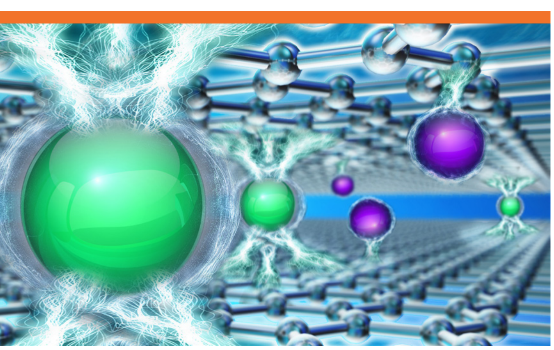
Early Career Opportunities: Students and Postdoctoral Fellows

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	FY16	FY17	FY18	FY19	FY20
Students supported by LDRD	102	127	138	160	101
Percentage of all students	19%	22%	22%	23%	18%

Postdoctoral Researchers	FY16	FY17	FY18	FY19	FY20
Postdoctoral researchers supported by LDRD ≥10% of their time	107	137	167	170	208
Percentage of all postdoctoral researchers	39%	44%	54%	57%	63%
LDRD postdoctoral researchers converted to full staff	25	31	52	46	60
Percentage of all conversions	69%	53%	71%	68%	77%

Principal Investigator: Patrick Campbell
LDRD Project: Selective Removal of Ions from Aqueous Solutions



Artist rendering of the cation adsorption in a graphene network, the process on which capacitive deionization is based.

Summer students explore ways to optimize the performance of desalination technology

A group of summer students were able to dive into research aimed at increasing access to fresh water, as part of an LDRD-funded project that explored methods to improve the performance of capacitive deionization (CDI), a desalination technology. They participated in experiments exploring how to overcome barriers that can limit the performance of CDI technology, which uses cyclic charging and discharging of electrodes to selectively remove ions and reduce the salinity of water.

One undergraduate summer student, Helen Kuo, also was the lead author of a journal article published in Environmental Research: Water Research & Technology. According to Kuo, "We detailed new methods for separating contact resistance vs. electrode resistance, and we provided an explanation of poorly understood impedance features. These measurements will help us design more efficient CDI cells."

After working with her mentor to design the experiments, Kuo built a series of CDI cells with different current-collector materials, including graphite and titanium, and used two- and four electrode measurements to decouple contact resistance from electrode resistance. In doing so, the team addressed a long-standing mystery in interpreting impedance measurements in porous electrochemical systems, presented a novel way to characterize current-collector degradation, and identified the top limitations of their own cell design.

LLNL scientist and co-author Steven Hawks said the talent and productivity of the undergraduate students were key to the project's success. The work has significant implications for scale-up of CDI systems and future improvements of cell design.

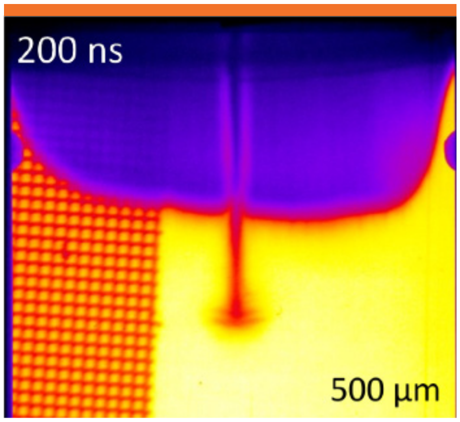
Doctoral fellow improves codes used to simulate interactions between particles moving at high velocities

Principal Investigator: Alison Saunders

LDRD Project: Metal Ejecta: Transport, Interaction, and Recollection

Doctoral fellow Marco Echeverria is part of an LDRD-funded research team exploring interaction between ejecta—particles ejected from a material's surface following shock-driven processes that cause the micron-sized particles to travel at high velocities. For example, they are studying metal ejecta generated from copper and tin material samples during high-power laser experiments, comparing how the mass, velocity, and material phase influences particle interaction.

According to LLNL physicist Alison Saunders, principal investigator of the LDRD project, gaining a better understanding of ejecta interactions has a broad range of applications, such as spacecraft shielding, cold-spray welding, additive manufacturing, and understanding material strength at small scales.



Radiography image of an ejecta microjet traveling downward (with the laser drive coming from above), captured during experiments conducted by LLNL's research team as part of their efforts to characterize ejecta interactions.

Echeverria's most recent role on the project focused on improving hydrodynamics codes used to model phenomena that occur during high-energy experiments. "It's challenging to simulate the material's microstructure at a large scale," he explained. "By feeding better experimental data into the hydrocodes, combined with data from molecular dynamics, scientists can conduct more realistic simulations at experimental scales."

Echeverria is a GEM fellow, sponsored by LLNL. The National GEM Consortium enables qualified students from underrepresented communities to pursue graduate education in science and engineering. Echeverria is earning a doctoral degree in materials science and engineering from the University of Connecticut and had originally planned a career in academia. After experiencing the research environment at LLNL, his plans shifted.

"I really like the close connection between experimental work and modeling that's possible in a national lab research environment," Echeverria said. "It's exciting to be able to reverse-engineer simulation codes based on experimental results."

"We are thrilled that Marco chose to be part of this research team," said Will Evans, who leads LLNL's Physics Division. "Sponsoring GEM fellows is an important part of our efforts to attract a diverse group of talented young physicists to the Laboratory and expand collaborations in the broader physics community."

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 of time, 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 2020, 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		
	FY18	FY19	FY20	FY11–15 (5 yrs)	FY16–20 (5 yrs)	FY00–20 (21 yrs)
Total APS awards	4	6	4	25	21	94
Awards with LDRD roots	4	5	4	24	20	87
% with LDRD roots	100%	83%	100%	96%	95%	93%
Average years from first LDRD experience	18.0	15.6	20.8	13.6	18.2	12.7

TRACING IMPACT TO LDRD ROOTS

Throughout this section, we mention "LDRD roots." There is often a lot of discussion with principal investigators 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.

2020 APS Fellows at LLNL

Four LLNL scientists were selected as 2020 fellows of the American Physical Society. These new fellows represent a range of physics expertise, including laser-plasma physics, magnetic-fusion plasmas, condensed-matter physics, and theoretical and computational understanding of plasma interactions.

RICHARD BERGER

"I am grateful to my colleagues who nominated me, and I am very pleased to receive this recognition."

Richard Berger, a theoretical plasma physicist at LLNL, was recognized for his pioneering vision regarding the crucial theoretical and computational understanding of plasma interactions with intense light and other high-energy-density plasmas. He joined LLNL in 1991, and his LDRD-funded work reflects his research focus on fluid and kinetic simulation of laser-plasma interactions, as well as multi-fluid hydrodynamics and kinetic instabilities driven by interpenetrating plasma flows.

LAURENT DIVOL

"I am honored to have been selected. I feel this fellowship is a recognition of my contributions to many ICF projects—an opportunity that is truly unique to national labs."

LLNL physicist Laurent Divol was selected as an APS fellow for fundamental contributions to laser-plasma physics in hohlraums and other high-energy-density experiments, and for leadership in the design of high-yield deuterium-tritium experiments. Divol joined LLNL in 2001 and works on many projects related to inertial confinement fusion (ICF), with a focus on research involving lasers and plasmas. His LDRD roots include a project in which he developed a novel scheme for guiding laser beams in plasmas.

MAX FENSTERMACHER

"I'm very grateful to have worked with great team members who were key to the new physics understanding obtained through our research, which was cited in this award."

Plasma physicist Max Fenstermacher was recognized for his experiments and modeling related to understanding tokamak divertor detachment, as well as the characterization and control of edge-localized modes (ELMs) with resonant magnetic perturbations in magnetic-fusion plasmas. He started his career at LLNL in 1983, and since 1994 he has served as a member of the LLNL experimental team at the DIII-D National Fusion Facility in San Diego. His LDRD-funded research includes studies of heat loads in tokamaks, including measuring and analyzing ELM behavior with diagnostics on the two largest U.S. tokamaks.

ART NELSON

"I am truly honored to be selected as an APS fellow, and I appreciate my many colleagues in the Peak Brightness Collaboration for supporting my nomination."

Art Nelson, an expert in condensed-matter physics, was recognized for his outstanding contributions to the development of soft x-ray and free-electron laser analytical platforms and pump-probe techniques applied to understanding ultrafast surface phenomena and extreme states of matter. He has worked at LLNL for 22 years, and his LDRD-funded work aligns with his research focus on studying surface catalytic reactions and designing novel materials for energy applications.

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. For the first time, as each institution issues its LDRD program report for fiscal year 2020, we are presenting a common set of long-term performance indicators, which include the content provided below.

Distinguished Member of the Technical Staff

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

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

As presented in the table 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.

OVER THE LAST 20 YEARS, approximately half of LLNL's R&D 100 Awards had roots in the LDRD Program.

History of DMTS Awards at Lawrence Livermore National Laboratory

	Single-Year Statistics			Multi-Year Statistics		
	FY18	FY19	FY20	FY11–15 (5 yrs)	FY16–20 (5 yrs)	FY11–20 (10 yrs)
Total DMTS awards	4	6	None	34	14	48
DMTS with LDRD roots	4	6	N/A	27	14	41
% with LDRD roots	100%	100%	N/A	79%	100%	85%
Average years from first LDRD experience	23.8	17.5	N/A	18.1	21.1	19.1

History of R&D 100 Awards at Lawrence Livermore National Laboratory

	Single-Year Statistics			Multi-Year Statistics		
	FY18	FY19	FY20	FY11–15 (5 yrs)	FY16–20 (5 yrs)	FY00–20 (21 yrs)
Total R&D 100 awards	0	4	1	20	15	89
Awards with LDRD roots	N/A	2	0	11	4	45
% with LDRD roots	N/A	50%	0%	55%	27%	51%
Average years from first LDRD investment	N/A	12.0	N/A	6.5	8.8	6.2

Members of the LLNL team who developed the Scalable Checkpoint/ Restart Framework 2.0, an innovative technology that received an R&D 100 Award in 2019 and has with roots in a 2010 LDRD project.

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 244 projects in fiscal year 2020. 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.

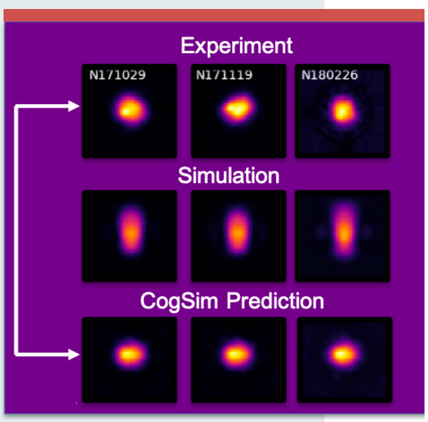
Predictive capabilities integrate cognitive simulation tools with complex experimental data

Principal Investigator: Brian Spears

LDRD Project: Learning-Based Predictive Models: A New Approach to Integrating Large-Scale Simulations and Experiments

Predictive simulation capabilities play a key role in many high-priority missions, including nuclear security, critical infrastructure protection, and biosecurity. The accuracy of these predictive models relies on the ability to compare simulation results with experimental data. However, in many of these mission-critical research areas, it has been extremely challenging to incorporate the full scope of available experimental data into predictive models.

In an LDRD-funded project, which is part of the Laboratory's cognitive simulation initiative, researchers are developing advanced machine-learning techniques that will combine our rapidly expanding simulation capabilities with our precision empirical data sets. These learning-based predictive techniques can better align simulations with experimental data, improving the accuracy and efficiency of simulations.



LLNL's new cognitive simulation tool ingests data from past experiments to predict future experimental outcomes, providing data that are far closer to true experimental observations than what can be obtained by previous modeling techniques

According to Brian Spears, an LLNL physicist who leads the research team, investigators have developed new deep-neural-network technologies designed to make full use of available data sets from experiments. The novel technology is capable of handling extensive collections of multimodal experimental data, including images, vector-valued data, time histories, and scalar measurements.

These transformative predictive capabilities can speed up extremely complex calculations and compare varied data sources efficiently, without requiring a scientist to scan tremendous amounts of data. The interdisciplinary team that developed this exciting new technology includes experts in machine-learning architectures, deep learning, data harvesting, and intelligent data sampling.

"The ability to combine multiple, scientifically relevant data streams will open the door to a wide range of new types of analyses," explained Spears. "It will allow us to extract information from our most valuable experimental and simulation data sets that has been inaccessible until now. Fully exploiting this information, in concert with a new suite of related cognitive simulation tools, will lead to improved predictive models."

These new predictive capabilities based on machine learning have already been integrated into multiple programs at LLNL, ranging from atmospheric release modeling to pathogen spread modeling.

Additive manufacturing of metals for mission-critical applications—one drop at a time

Principal Investigator: Jason Jeffries

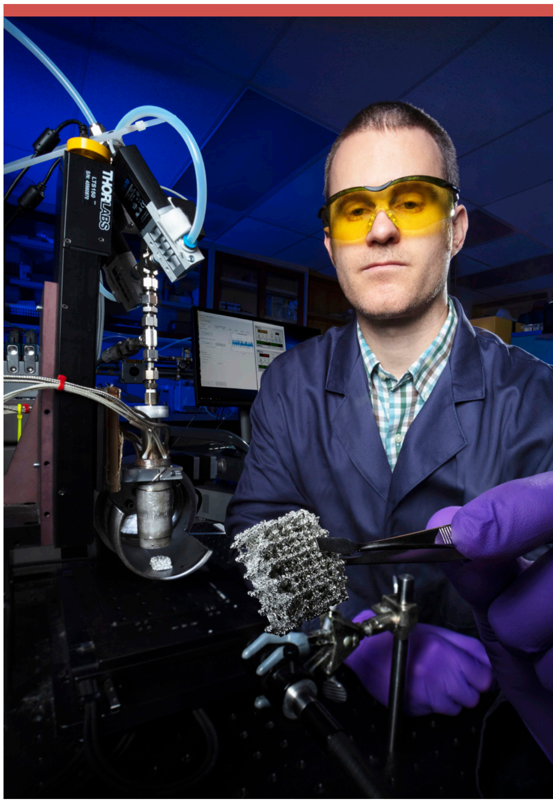
LDRD Project: Developing and Characterizing New Tools for Actinide Processing Science

The ability to engineer mission-critical metal parts using advanced manufacturing techniques continues to play a key role in research at LLNL. Existing three-dimensional (3D) printing methods, which build precise parts in sequential layers, do not work well with all types of metals. Recognizing the need to design and deliver metal parts with tailored properties, including parts made from actinide materials, a research team at Livermore adapted a 3D-printing technique known as liquid metal jetting (LMJ) and explored how it can be used to produce parts with the structure and tailored properties needed to meet the needs of national security stakeholders.

According to LLNL physicist Jason Jeffries, who led the LDRD-funded research team, LMJ eliminates problems typically found with selective laser melting (SLM) techniques. "Selective laser melting limits the types of metal feedstocks that can be used because many metals become highly reactive when they are converted to a powder," explained Jeffries. In addition, the use of fine powders can cause spattering, which may inadvertently contaminate a part, or the powder can get trapped inside a part and vaporize, resulting in an unwanted void in the finished build.

"Liquid metal jetting is a much gentler and more localized process," said Jeffries. And because LMJ uses raw feedstock, it can bypass the extra processing step of converting it into powder.

LLNL's multidisciplinary effort to enhance LMJ capabilities included researchers in physics, materials science, mechanical engineering, and computational engineering. They explored how to control tiny droplets of metals, heated above their melting temperatures, which subsequently fall onto a substrate to produce 3D parts from a stack of two-dimensional digital patterns. Upon solidification, each layer of jetted droplets acts as a new substrate onto which new droplets are dispensed to create the adjacent layer. As the droplet-on-demand process repeats, complex 3D geometries can be printed with extremely fine detail.



Livermore engineer Nick Watkins, architect of LLNL's specialized liquid metal jetting (LMJ) machine, displays an LMJ-manufactured metal part.

The team studied how various techniques affect the build speed and quality of parts. For example, they developed and tested a machine with two different printing modes—a continuous stream and a droplet-on-demand process, which produces discrete droplets ejected from a nozzle. By combining the capabilities into a single machine, an object can be manufactured using both modes, offering the speed of a continuous material stream, and the resolution offered by the droplet-on-demand mode.

The LDRD-sponsored research advanced the state-of-the-art in advanced manufacturing with actinides and other metals, improved scientists' understanding of actinide alloys and high-temperature actinide synthesis, and enhanced LLNL expertise in actinide science.

The team also studied how to modify the process to obtain optimal mechanical properties. For example, they analyzed how much of the underlying structure should melt as the molten drop bonds to the metal underneath it. In addition, they explored ways to control the cooling rate of the microstructure by modifying the droplet ejection velocity, size, and frequency.

Researchers demonstrated that the technique can be used to produce metal parts with unique shapes, structures, and properties that are not possible with conventional machining, casting, or 3D-printing methods.

LDRD projects explore medical countermeasures to mitigate the impact of COVID-19

Related LDRD Projects

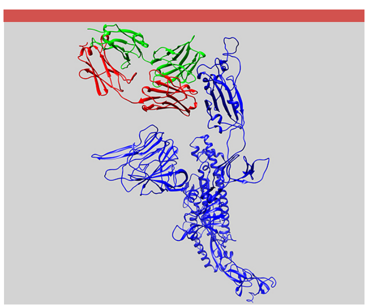
Identifying Potential Antiviral Small Molecules Against COVID-19 | PI: Felice Lightstone

Active Learning for Rapid Design of Vaccines and Antibodies | PI: Tom Desautels

Rapid Computational Identification of Therapeutic Targets for Pathogens | PI: Jonathan Allen

Building a Computational and Experimental Rapid Response Pipeline to Counter the COVID-19 Outbreak and Emerging Biothreats | PI: Brent Segelke

A Deep Bayesian Active Learning Framework for Temporal Multimodal Data | PI: Priyadip Ray



Computer model of the 3D structure of an antibody candidate (green and red) with the SARS-CoV-2 spike protein in blue.

Livermore's LDRD program invests in research aimed at meeting some of the nation's most difficult challenges. Shortly after the COVID-19 pandemic emerged in early 2020, these internally directed funds enabled LLNL to rapidly launch new projects and redirect the focus of existing projects to help the nation respond to the pandemic.

According to Doug Rotman, who leads the LDRD program at Livermore, "We had several scientists contact us with ideas regarding how they could help our Laboratory respond to the national COVID challenge, including emerging needs related to therapeutic targets and designs. Working closely with science leaders across LLNL, the LDRD program rigorously and quickly evaluated proposals and approved funding needed to start work."

The LDRD-sponsored projects leveraged LLNL's capabilities in high-performance computing, simulation, and data science—combined with Livermore's expertise in bioscience and bioengineering—to identify risk factors for COVID-19 patients and accelerate development of medical countermeasures.

LLNL combines bioinformatics expertise and supercomputing resources to explore antiviral drug design

Soon after the pandemic was recognized as a global crisis, leaders of three LDRD-funded projects quickly expanded the scope of their projects, focusing on efforts to identify new antibodies and antivirals that could treat a COVID-19 infection.

Armed with the predicted protein structure of especially important parts of the viral replication machinery and a handful of antibodies known to bind and neutralize SARS-CoV-1 (a similar coronavirus that causes Severe Acute Respiratory Syndrome), researchers used LLNL's high-performance computing platforms and artificial intelligence resources to virtually screen antibodies capable of binding to SARS-CoV-2 virus receptors and neutralizing them. Their novel approach integrated bioinformatic modeling and molecular simulations, driven by a machine-learning algorithm, to identify antibody candidates.

These techniques provided the team with the speed and scalability needed to search and evaluate huge numbers of possible antibody designs and reduce the possibilities to 20 initial sequences predicted to target SARS-CoV-2. This approach sped up the process considerably, and enabled scientists to focus their search on areas they might otherwise have overlooked—in the appropriate design space.

"Being able to rapidly estimate antibody structures makes it possible to follow up on promising predictions as they emerge," said data scientist Tom Desautels, who leads one of the LDRD-funded projects. "Searching a design space of this size wouldn't be feasible without powerful computing resources because the volume of decisions is too high."

Experimental validations of top candidates improve countermeasure development

The virtual screening of millions of antibody and antiviral candidates made it possible for the team to identify an initial set of promising compounds in just a few weeks. The next step involved a team of LLNL experts in virology, immunology, and molecular biology, who synthesized and validated the efficacy of top candidates through experiments—another example of work that was quickly launched by expanding the scope of an existing LDRD project.

Using binding assays and biolayer interferometry technology, the experimental team conducted precise measurements to test how well the molecules bind to their target. They used these measurements to rank therapeutic candidates and further narrow the pool of computationally identified candidates with the antiviral properties needed to fight this disease. The experimental team tailored their research to ongoing computational efforts, so that the two aspects of the research worked synergistically, with validated results feeding back into predictions.

Multimodal machine-learning tools predict risk factors for COVID-19 patients

Investigators of another LDRD-funded project also shifted their focus after the pandemic began. A team of computational scientists was studying ways to use multimodal machine learning to fuse information from disparate sources and learn the underlying temporal structure of the data. They had already been exploring ways to apply machine-learning tools to existing medical datasets in order to more effectively predict clinical outcomes, and they realized they could adapt this work to conduct predictive risk analyses for COVID-19 patients.

Using the dynamic modeling framework they had started developing, the team fused genomic data regarding virus mutations with medical datasets regarding microbes present in clinical samples obtained from COVID-19 patients. They are now collaborating with data science experts at LLNL to create a diagnostic-testing knowledge base that the research community can use to predict the variables associated with COVID-19 disease progression. The data repository will help medical providers detect unforeseen, potentially actionable changes to a patient's health and identify optimal treatment options.

Diagnostic tool adapted to screen for COVID-19 co-infections

LDRD-funded research often focuses on innovative solutions with a broad range of potential applications. One example of this ability to tailor technology initially developed with LDRD funds involves a diagnostic tool known as the Lawrence Livermore microbial-detection array (LLMDA), developed in 2008. This high-throughput, nucleic-acid detection technology can simultaneously analyze and identify up to 12,000 microbial species in a single test.

LLNL scientists adapted LLMDA to analyze nucleic acids extracted from COVID-19 oral and nasal samples and identify the presence of other pathogens. Their work involved designing a unique COVID-19 signature that could be incorporated into the existing LLMDA technology to detect the presence of the SARS-CoV-2 virus. They validated the new capability using LLMDA to analyze samples that had already tested positive for COVID-19 using more traditional diagnostic methods, and then looked for the presence of other pathogens in the samples. They were able to identify several types of co-infections, such as Influenza A and Streptococcus pneumoniae.

The team anticipates that collecting this co-infection data can help scientists better understand how the presence of other pathogens may affect a person's susceptibility to COVID-19 infection, as well as how they respond when infected with the SARS-CoV-2 virus.

Principal Investigator: Lara Leininger

LDRD Project: Unlocking the Mysteries of High-Explosive Science

This innovative research will inform future development of detection technologies for nonproliferation missions, as well as interdiction technologies for nuclear counterterrorism and other national security missions.

Livermore scientists conducted the first-ever laser shot with explosives, providing key experimental data that can be used to validate predictive models and expand experimental capabilities in high explosives. This illustration depicts the experiment, showing the laser impacting a thin square of the HE material (shown in yellow), and the solid-carbon products (shown in black) that resulted from the chemical reaction.

Unprecedented experiments explore the mysteries of high explosives

Unlocking the mysteries of high-explosive chemistry may hold the key to addressing a range of mission-relevant challenges, including nonproliferation and counterterrorism. During an LDRD-funded research project that recently concluded, LLNL scientists moved beyond computational predictions regarding the behavior of high explosives. They obtained direct measurements of chemical reactions involving an insensitive high explosive—data that is unprecedented in high explosive (HE) science.

The research team conducted the first-ever experiment of this kind, using the world's most energetic laser to study a high-explosive sample. During their experiments at LLNL's National Ignition Facility (NIF), investigators captured novel diagnostic data that will help scientists better understand and predict HE behavior.

According to Lara Leininger, director of LLNL's Energetic Materials Center (EMC) and principal investigator for this LDRD project, "The laser shot is the first in a series of experiments that will transform the Lab's understanding of high explosives by producing never-before-captured experimental data quantifying the response of laser-driven high explosives during reaction." They captured detailed, temporally and spatially resolved data regarding the evolving chemistry of a reacting insensitive high explosive.

These expanded diagnostic capabilities will allow LLNL to investigate the structure of HE detonation products during the detonation, while also helping to validate predictive models that play a key role in understanding HE detonation and safety.

During the first phase of the three-year project, which started in 2017, the multidisciplinary team developed novel diagnostic techniques to measure in-situ, dynamic, laser-driven, high-explosive reactions. Their first experiment took place at LLNL's Jupiter Laser Facility.

According to LLNL physicist Jon Eggert, who led the project's high-energy-density experiments, the team was able to adapt an existing diagnostic platform, known as TARDIS (TARget Diffraction In Situ), to conduct the experiments. "It was gratifying to see that a platform we developed for very different scientific and programmatic applications, including its dual-probe and large spot-size options, could be used in this new research space," said Eggert.

In the second phase, they evaluated concepts during a series of shots at the Omega Laser Facility at the University of Rochester. They also investigated target preparation, configuration, and diagnostic setups.

The capstone phase of the project was performed at NIF, integrating the techniques developed in the first two phases with NIF's advanced diagnostic systems, which enabled the team to extract the required experimental data.

The sample used in the NIF shot consisted of a non-detonable quantity of less than 7 milligrams of single-crystal TATB (1,3,5-triamino-2,4, 6-trinitrobenzene), a HE with low sensitivity to external stimuli such as friction, pressure, temperature, impact, or spark.

According to Samantha Clarke, lead scientist for the experimental work at NIF, the team used the facility's long laser drive, coupled with two x-ray probe beams on the same target, to produce clear evidence of the formation of products in less than 50 nanoseconds. The experiment captured a time evolution of products under shock compression exceeding 150 gigapascals (1.5 million times Earth's atmosphere).

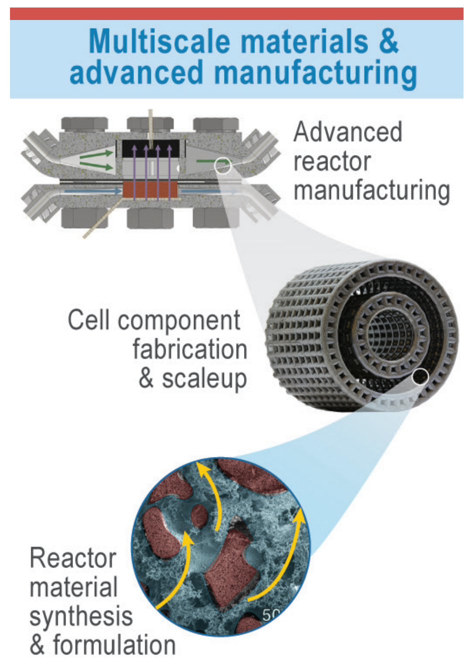
Modular electrochemical reactors efficiently convert carbon dioxide into valuable chemicals

Principal Investigators: Eric Duoss and Sarah Baker

LDRD Project: Manufacturing Molecules for the Carbon Economy

An LDRD-funded team of scientists and engineers developed a new electrochemical reactor paradigm in an effort to fundamentally rethink how chemical reactors are designed, making them smaller, more energy efficient, and more versatile. They also wanted to create an innovative new approach that transforms carbon dioxide (CO_2) harvested from the atmosphere into a valuable resource—industrial chemicals, polymers, and other useful compounds.

Much of the chemical-reactor technology in use today involves the use of energy-intensive thermochemical reactors, with an enormous infrastructure and high capital and operating costs. Through several LDRD research projects, including one that wrapped up recently, investigators developed a prototype electrochemical reactor that uses CO_2 as the reactant and converts it into multi-carbon molecules, such as ethylene and ethanol. It is small (with an electrode that measures just 1 square centimeter), and it uses a modular platform that can scale up for industrial settings.



LLNL's versatile electrochemical reactor design incorporates several innovative capabilities, such as 3D-printed components with the microstructure needed to control the catalyst environment, and the ability to tailor its performance to specific operating environments—enabling the reactor to efficiently transform carbon dioxide harvested from the atmosphere into valuable chemicals, such as ethylene.

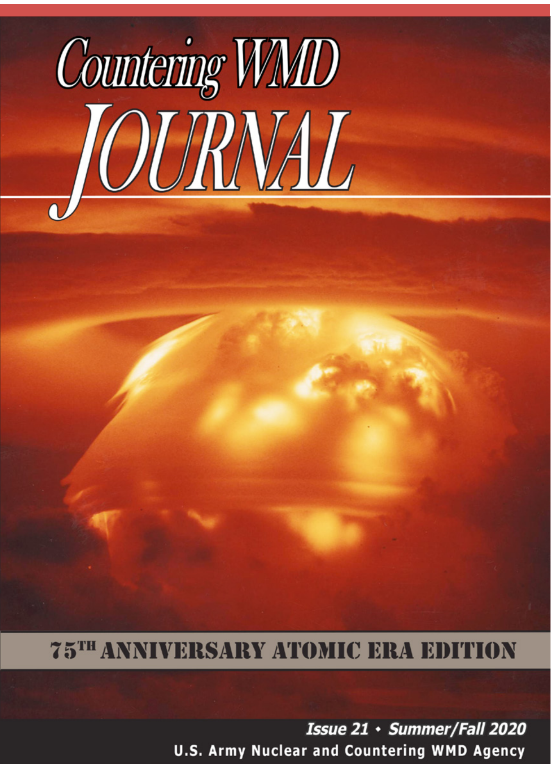
The research team integrated computational design, engineering, and materials science to refine the reactor model, along with three-dimensional additive manufacturing techniques, to produce reactor components that offer the microstructure needed to control the catalyst environment. Leveraging the versatility and precise control offered by the additive manufacturing techniques, they can speed up the process to produce electrochemical cells and reactors, and tailor them to specific operational variables.

LLNL materials engineer Eric Duoss and chemist Sarah Baker led the LDRD-sponsored research team that developed the reactor design and engineered the prototype. Baker is also partnering with Duoss to investigate scale-up of the technology through industry and university collaborations.

The smaller, customizable reactor design will enable a transition from expensive, large-scale chemical plants to distributed, more economical chemical reactor networks.

Principal Investigator: Kim Knight

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



A special edition of a U.S. Army journal features work by LLNL scientists, who analyzed historical data regarding near-surface nuclear events.

LLNL research highlighted in journal edition commemorating the dawn of the nuclear age

The summer of 1945 marked a turning point in history, with the world's first nuclear detonations. When editors of a U.S. Army journal decided to publish a special edition commemorating the 75th anniversary of these historic events, they contacted LLNL nuclear forensic scientist Kim Knight, seeking possible articles for a special issue of the Countering Weapons of Mass Destruction (WMD) Journal.

Knight has been studying historic fallout from near-surface nuclear events for many years, and at the time the editors contacted her, she was already working with more than 25 LLNL investigators on an LDRD-funded research initiative studying how different environments affect nuclear explosions. When the special edition of the journal was released in late 2020, 5 of its 15 articles were written by LLNL scientists.

"The timing of our work fit perfectly for their request," said Knight. "It was a great way to bring awareness of our work to a broad audience, including our hypothesis that interaction of the local environment with a nuclear detonation changes how the fireball evolves."

Knight's research team combined computational and experimental approaches to create an informed framework capable of modeling nuclear detonations, taking into account how the environment contributes to the physical and chemical evolution of the fireball plasma and resultant debris. Investigators analyzed historical films of nuclear tests and studied nuclear debris; modelers built into simulations of nuclear detonations the key physics and chemistry needed to account for time-dependent entrainment; and experimentalists studied chemical speciation and early debris-formation processes through laser interactions with matter and plasma chemistry.

"The experimental work informs the chemistry that we need for the models, which we're grounding in historical data from films and debris," Knight explained.

The research continues to play a key role in expanding LLNL expertise in fallout science, while supporting NNSA's nuclear threat reduction goal.

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 2020, attesting to the exceptional talents of these researchers and underscoring the vitality of Livermore's LDRD program.

Fellows

WILLIAM PITZ

Fellow, Society of Automotive Engineering

The Society of Automotive Engineering selected physicist William (Bill) Pitz as a fellow in recognition of his significant impact on the development of mobility technology through leadership, research, and innovation. His research at LLNL includes studies of combustion phenomena in various types of engines.

J. CHANCE CARTER

Fellow, Society of Applied Spectroscopy

Chance Carter was selected as a fellow of the Society of Applied Spectroscopy for his exceptional contributions to spectroscopy. His achievements include development of spectroscopic-based analytical methods and systems, remote and standoff Raman and infrared spectroscopy, and fiber-optic sensors.

PETER BEIERSDORFER

Fellow, American Astronomical Society

Peter Beiersdorfer's selection as a fellow of the American Astronomical Society (AAS) builds on the recognition he received with his previous Laboratory Astrophysics Prize from AAS. During his career, Beiersdorfer has pioneered techniques to reproduce conditions in the sun's atmosphere, interstellar space, the centers of galaxies, and on comets. A major focus of his research is characterizing atomic and molecular diagnostics as revealed by their x-ray spectra. His studies of emissions from the inner electron shells of iron, oxygen, neon, silicon, and sulfur are used to interpret the physical conditions in astronomical environments near and far. His work on x-ray emission from charge exchange revealed the importance of this process in cometary atmospheres.

FÉLICIE ALBERT

Kavli Fellow, National Academy of Sciences

As a new elected Kavli fellow of the U.S. National Academy of Sciences, Félicie Albert was invited to present a poster at the annual U.S. Kavli Frontiers of Science symposium, where she discussed her research on using plasmas produced by intense lasers as particle accelerators and x-ray light sources. Albert currently serves as the deputy director of LLNL's High Energy Density Science Center. She is a fellow of the American Physical Society and a senior member of the Optical Society of America.

"I am really honored to have been selected as a Kavli fellow and to have been invited to the U.S. Kavli Frontiers of Science Symposium. The event was a great way to showcase the work we do at LLNL using lasers."

BRONIS DE SUPINSKI

Fellow, Institute of Electrical and Electronics Engineers

The Institute of Electrical and Electronics Engineers named Bronis de Supinski as a fellow in recognition of his leadership in the design and use of large-scale computing systems. As chief technology officer for Livermore Computing, he is responsible for formulating LLNL's large-scale computing strategy and overseeing its implementation. His research interests include compilers, tools, and runtime systems, particularly programming models. He also chairs the OpenMP Language Committee.

"I am pleased to be elevated to an IEEE fellow. I am grateful to my colleagues for their essential contributions to the research and system development that are the hallmark of my achievements. These achievements have enabled me to reach a goal that I set for myself many years ago—to be a world-leading computer scientist."

CAROL WOODWARD

Fellow, Association for Women in Mathematics

The Association for Women in Mathematics (AWM) named computational scientist Carol Woodward a fellow, recognizing her commitment to supporting and advancing women in the mathematical sciences. A computational mathematician in LLNL's Center for Applied Scientific Computing since 1996, Woodward's research focuses on nonlinear solvers and time-integration methods and software. She is part of the DOE FASTMath SciDAC Institute project to improve numerical software for use in DOE applications. She is developing integration methods for transmission power grid simulation as part of DOE's advanced grid modeling program and for climate simulations as part of the greater SciDAC program.

"Being selected as an AWM fellow is special to me. Promoting the amazing work that women do in mathematics, as well as encouraging equal treatment for women, have been causes I strongly support and have worked hard to develop. The AWM does so much amazing work in support of women and girls in mathematics, and I find it a humbling honor to be recognized by them."

Other Awards

Bert Bolin Award, American Geophysical Union

Atmospheric scientist Benjamin Santer was honored with the American Geophysical Union's 2020 Bert Bolin Award, recognizing groundbreaking research or leadership in global environmental change. Santer's work focuses on climate model evaluation, the use of statistical methods in climate science, and the identification of natural and anthropogenic "fingerprints" in observed climate records. His early research on the climatic effects of combined changes in greenhouse gases and sulfate aerosols contributed to the historic "discernible human influence" conclusion of the 1995 IPCC report. His recent work attempts to identify anthropogenic fingerprints in a number of climate variables, such as tropopause height, atmospheric water vapor, the temperature of the stratosphere and troposphere, oceanic heat content, and ocean-surface temperatures in hurricane formation regions.

"This award has deep personal meaning for me. I've never forgotten Bert Bolin's kindness and encouragement. The lecture will be an opportunity to pay tribute to a great man and a great scientist."

John Dawson Award, American Physical Society

Three LLNL scientists received the 2020 John Dawson Award for Excellence in Plasma Physics Research from the American Physical Society. The team generated Weibel-mediated collisionless shocks in the laboratory, informing a broad range of energetic astrophysical scenarios, plasma physics, and experiments that use high-energy and high-power lasers at plasma science facilities.

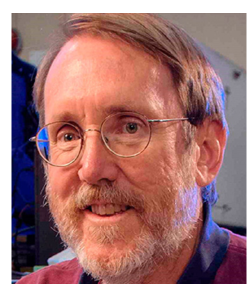
Collisionless shocks have been of intense scientific interest for more than half a century. They are a fixture in astrophysical plasmas and are believed to generate and amplify magnetic fields in the universe and accelerate particles as a source of cosmic rays in a variety of objects, including colliding galaxies, supernova explosions, and gamma-ray bursts.

HYE-SOOK PARK

"It is a great honor to receive this award. I truly appreciate all the team members and the fact that our devotion to great science has been recognized. I am thrilled to be a part of the work that solved a small piece of the puzzle of supernova explosions."

DMITRI RYUTOV

"Being a theorist, I enjoy working on projects where theory is closely coupled to an ongoing experiment and helps in the decision making. It was a great privilege for me to work with outstanding LLNL experimentalists. We have made one more step toward a better understanding of the processes driven by supernova explosions and other energetic events occurring in the universe."



JAMES STEVEN ROSS

"The idea of generating collisionless shocks was proposed ten years ago. It took a combination of improved physics understanding and new diagnostic capabilities to make this project successful. I find it very exciting that we can use the world's largest laser to create centimeter-scale plasmas that are relevant to astrophysical phenomena spanning light years."

DOE Office of Science Early Career Research Program Award

Two scientists who started their careers at LLNL as postdoctoral researchers and went on to lead LDRD-sponsored projects received DOE Early Career Research Program awards in FY2020. The program 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. Under the program, DOE national laboratory staff are awarded $500,000 per year for five years to further their research.

Microbiologist Erin Nuccio was selected for her research in fundamental systems biology, including her work studying the role of microbes in biogeochemical cycling processes using a systems biology approach.

Nuccio started at LLNL in 2013 as a postdoc studying plant-microbe interactions. She has served as a staff scientist since 2016, and is now studying how microbes control carbon and nutrient cycling in soil, with a focus on the rhizosphere and hyphosphere. She uses stable isotopes to track interactions and nutrient exchanges in the complex soil environment.

"Throughout my career, I have been keenly interested in the fundamental ecology of plant-microbe-soil interactions, and the role these relationships play in terrestrial carbon cycling and ecosystem sustainability," she said.

According to Nuccio, microbes engage in a lively 'cross-talk' that we are only beginning to understand through next-generation sequencing and metabolomics technologies. She looks forward to digging deeper into the fungal hyphosphere—an active site of soil nutrient cycling that we know little about, although it is a hotspot for fungal-bacterial interactions. For fungi that cannot decompose plant material by themselves, this is a key zone for nutrient foraging. Nuccio expects fungal interactions with the microbial community to be of paramount importance in this region.

LLNL scientist Erin Nuccio studies the role that plant-microbe-soil interactions play in terrestrial carbon cycling.

"It's an incredible honor to be selected for this award. It is a game-changer for building my research career at LLNL."

Physicist Federica Coppari, whose work on large laser facilities helped lead to the discovery of the atomic structure of superionic ice, was one of this year's award recipients. Coppari joined the Lab in 2011 as a postdoctoral researcher, and today she works on developing new experimental platforms to understand material behavior at extreme conditions, with a focus on the physics of phase transitions, melting, and material equations of state.

Giant lasers can compress and heat matter to extreme states. When combined with bright x-ray sources, they become very powerful tools for investigating the atomic-level structural changes induced by strong and ultrafast compression. Coppari's experiments are conducted in facilities such as LLNL's National Ignition Facility and at synchrotrons, where she uses ultrafast x-ray diffraction and extended x-ray absorption fine-structure diagnostics to characterize material properties at extreme conditions.

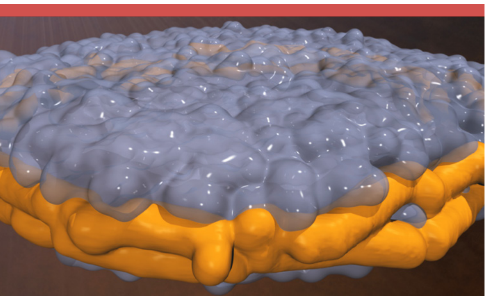
Coppari plans to use the DOE funding to investigate mixing and metastability in warm dense matter, with an emphasis on planetary constituent materials. "Matter deep inside planets is at extreme pressures and temperatures, and knowledge of its properties is key to improving our understanding of planetary formation and interior structure," she said. "It is extremely important to know how the different constituents mix (or unmix) when subjected to extreme conditions, although this is far from being understood."

"Pulling together ultrafast compression with x-ray and optical diagnostics, my research will investigate the transformations happening at extreme conditions of pressure, temperature, and timescale in complex, multi-component systems to obtain a better understanding of their mixing properties and pathways to phase transitions," Coppari explained.

Federica Coppari (left) and Erin Nuccio are recipients of the DOE Office of Science Early Career Research Program award.

Research Spotlight

Vaccine Delivery Platform Adapted to Fight Biothreats and Other Dangerous Pathogens



LLNL's NLP vaccine delivery platform can be fabricated with adjuvants and antigens that are tailored to respond to multiple types of pathogens. (Rendering by Tim Carpenter.)

Biotechnology developed through a series of LDRD-funded projects is now poised to serve as a versatile platform for drug and vaccine delivery across a range of health challenges. Initially developed to study membrane protein function, this tiny, yet highly powerful nanotechnology is being used to defend against biological threats. It is also being adapted to serve as a potent, safe, targeted vaccine delivery platform.

Tailored nanoparticle platform delivers customized vaccines

The biotechnology got its start in 2005 with a three-year LDRD-funded research project led by LLNL chemist Paul Hoeprich. According to Hoeprich, his research team explored ways to leverage research in cell membrane biochemistry to better understand the mechanics of drug transport into cells. "We brought these ideas together, developing our initial concept for a nanoscale drug delivery platform," said Hoeprich.

During LDRD-funded projects spanning more than a decade, investigators developed and tested the nanolipoprotein particle (NLP) platform, which can be tailored to activate the immune system against multiple pathogens. The platform's foundation consists of naturally occurring molecules that mimic cell membranes. They can self-assemble and provide a platform for connecting other biomolecules.

For example, scientists can attach adjuvants (molecules designed to boost vaccine potency) and antigens (molecules capable of inducing a specific immune response) to an NLP platform, making it possible to administer both types of molecules in a single controlled package aimed at responding to a specific type of pathogen. The disc-shaped platform measures between 8 and 25 nanometers in diameter—the ideal size to leverage natural pathways into cells, particularly immune cells relevant to vaccine delivery.

Rather than serving as a single-pathogen solution, the NLP platform provides the foundation to fabricate multiple types of vaccines. And since the particles are naturally present in the human body, vaccines produced using the NLP platform are less likely to result in toxicity.

Biodefense solutions

The initial focus of LLNL's research regarding NLP-based vaccines was their potential to protect military personnel and first responders against biothreat pathogens with no existing vaccines, or vaccines that require multiple doses to elicit a protective immune response.

As the technology matured through these initial LDRD investments, additional funding provided by the U.S. Defense Threat Reduction Agency (DTRA) enabled LLNL scientists to focus on ways they could use NLP technology to develop a vaccine capable of responding to one of the most infectious bacterial pathogens in existence, *Francisella tularensis*, the bacterium that causes tularemia. Although the pathogen is rare, it has a high mortality rate, even at low doses, and is considered to be a potential biothreat agent.

TIMELINE

2005 LDRD investments fund initial explorations of a new biotechnology to enhance vaccine development and delivery.

2011 LLNL investigators start exploring ways to use NLP technology to protect against biothreats and deliver cancer therapeutics.

2014 LLNL starts exploring use of NLP technology for subunit vaccines in collaboration with biotech company Synthetic Genomics.

2016 NIH funding supports development of a chlamydia vaccine using NLP technology. Follow on NIH funding in 2019 established a cooperative research center.

2017 NLP technology licensed by EVOQ Therapeutics for cancer immunotherapy.

2020 DTRA-funded research begins, focused on using NLP technology to develop and optimize a tularemia vaccine.

2021 LLNL initiates an industry collaboration to explore using NLP technology to develop a broad spectrum vaccine against coronavirus pathogens.

LLNL investigators are collaborating with scientists from the University of New Mexico to develop a multi-antigen vaccine capable of stimulating strong antibody and T-cell responses, providing protection against the bacteria, even when aerosolized. It uses the NLP delivery platform to co-deliver the tailored combination of antigens and adjuvants. They recently expanded their collaboration to include Tulane University as they explore ways to optimize the tularemia vaccine for clinical use and produce it at scale. Similarly, in 2011, the National Institutes of Health (NIH) provided funding for a collaborative research initiative, co-led by LLNL and Loyola University, aimed at developing an improved vaccine to protect against *Bacillus anthracis*, the causative agent of anthrax.

Public health applications

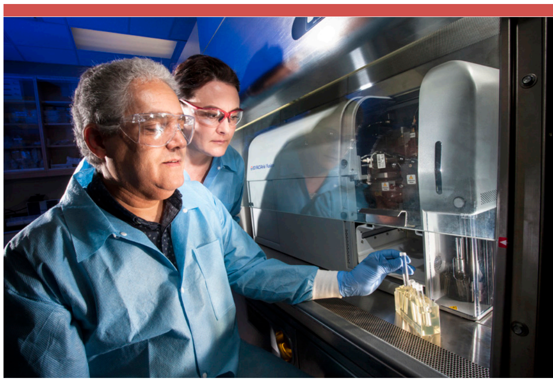
Biotechnology experts at LLNL continue to fine-tune the NLP technology, recognizing its potential to address other types of pathogens. For example, in 2016, with NIH funding, LLNL scientists collaborated with researchers at the University of California (UC), Irvine, to explore how NLP technology could be used to develop a vaccine that provides protection against chlamydia, the most common sexually transmitted pathogen in the world.

Building on this initial work, in 2019, NIH provided additional funding to establish a cooperative research center and expand these efforts. LLNL leads the center, which includes a multidisciplinary team of experts in immunology and nanotechnology from LLNL, UC Irvine, and UC Davis.
Together, they are exploring the most promising antigen formulas, as well as how to refine the NLP platform to effectively deliver the chlamydia vaccine.

Coronavirus vaccine development

The most recent application NLP technology involves the search for a broad-spectrum, universal coronavirus vaccine, capable of providing protection against coronavirus pathogens such as Middle East Respiratory Syndrome (MERS), Severe Acute Respiratory Syndrome (SARS), and SARS-CoV-2, the virus that causes COVID-19. With an LDRD investment in this new research, which launched in 2020, LLNL investigators are collaborating with ConserV Bioscience, a vaccine development company.

A broad-spectrum vaccine is a necessary next step to protect against continued mutations of SARS-CoV-2, as well as new coronavirus strains that become more virulent and pose a pandemic threat. The team will focus on designing a vaccine that targets regions of the virus proteins that are not susceptible to change, enabling it to provide protection as the virus mutates. In addition, researchers anticipate that the NLP platform will reduce the timeframe needed to develop new vaccines.



LDRD investments over more than a decade enabled LLNL scientists, including biologist Matt Coleman and immunologist Amy Rasley, to explore how NLP technology can be used to develop new vaccines and deliver cancer therapeutics.

Related LDRD Projects

PI Paul Hoeprich | Project 06-SI-003

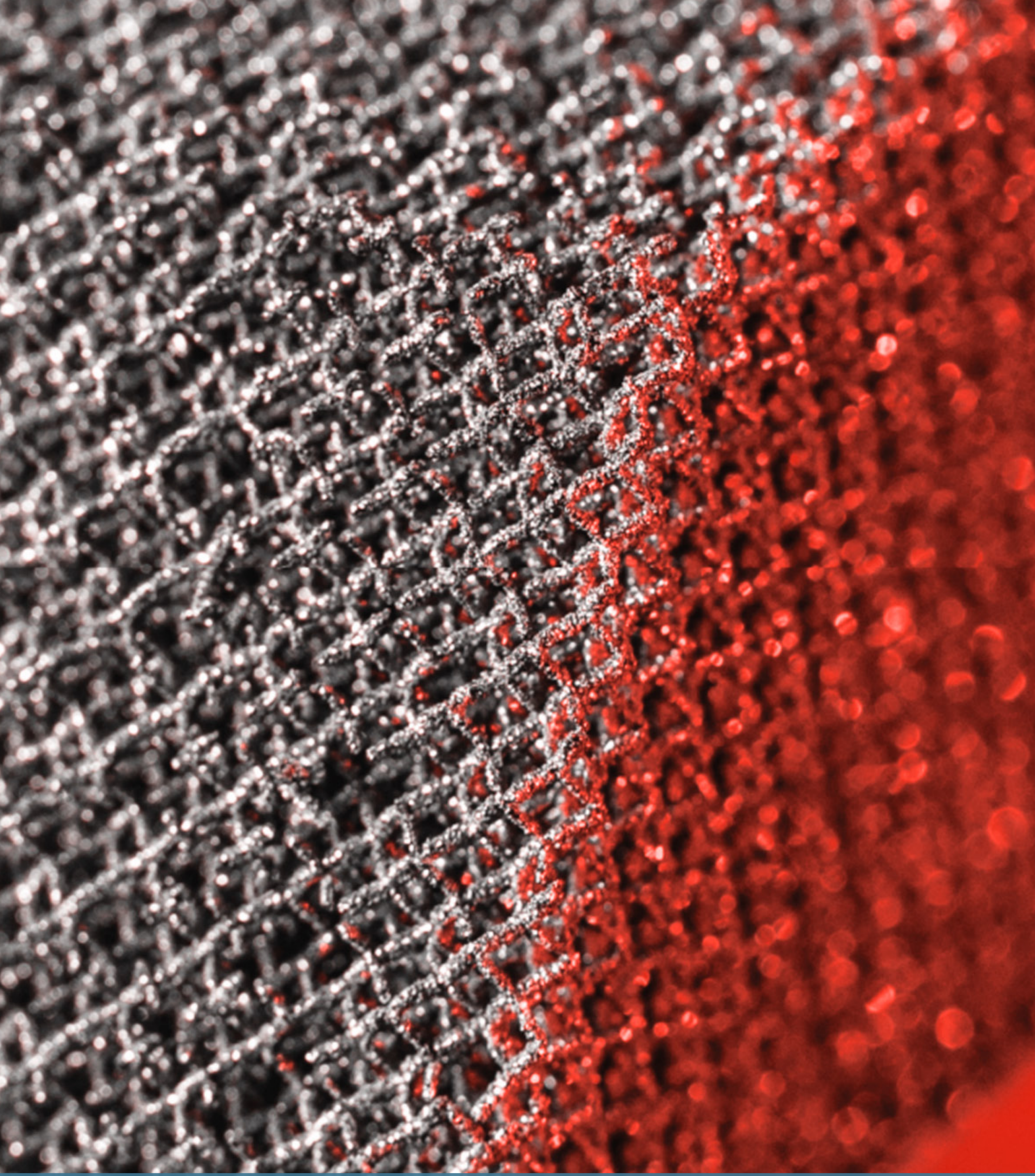
PI Craig Blanchette | Projects 09-LW-007 & 15-LW-023

PI Amy Rasley | Project 11-ERD-016

PI Nicholas Fischer | Projects 11-LW-015 & 20-ERD-004

PI Matthias Frank | Project 12-ERD-031

PI: Sean Gilmore | Project 17-LW-051



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