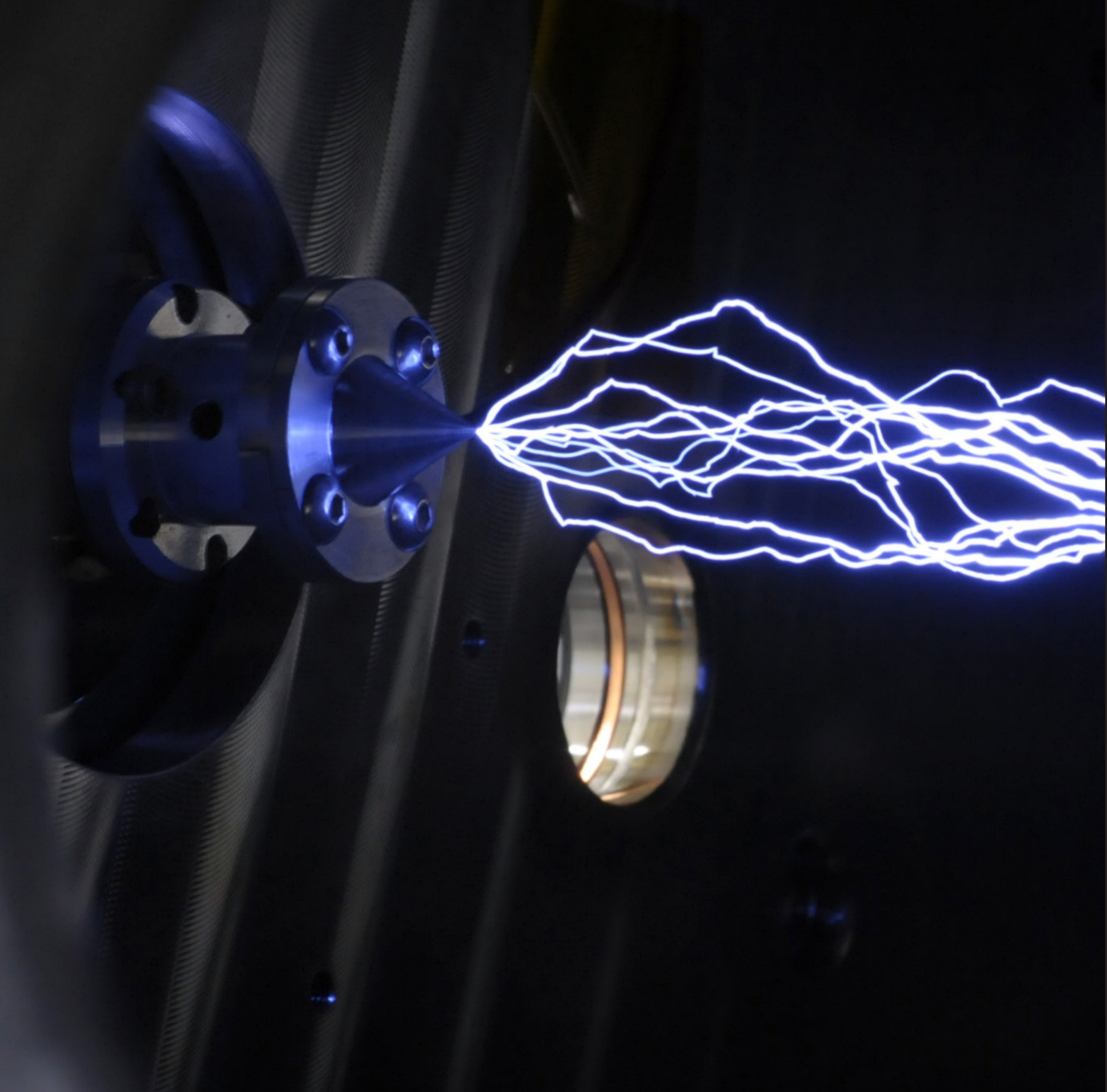
Los Alamos National Laboratory

Laboratory Directed Research and Development Program

FY24 Annual Progress Report



Los Alamos
NATIONAL LABORATORY

LDRD LABORATORY DIRECTED
RESEARCH & DEVELOPMENT

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LABORATORY DIRECTED
RESEARCH & DEVELOPMENT

FY24 Annual Report

Structure of this Report
The Laboratory Directed Research and Development (LDRD) Annual Report for fiscal year 2024 (FY24) is organized as follows:

Overview: A description of the LDRD program at Los Alamos National Laboratory (LANL), including the program's structure and objectives; a summary of the program's value; and highlights of outstanding program accomplishments.

The Annual Report is available at:
https://www.lanl.gov/engage/organizations/nnsa-directed-r-and-d/annual-reports

On the Cover
Cover Image: PHOENIX: Portable, High-efficiency, Orthovoltage ENergy, Imaging X-rays. This work, led by LANL researchers Scott Watson and Nicola Winch recently won an R&D 100 Award. The PHOENIX technology has roots in LDRD projects 20180037ER- MEXRAY (ME)chanical XRAY, PI: Scott Watson; and 20210540MFR- Megavolt Generator for Multiple-Pulse Hydrotesting, PI: Nicola Winch. Learn more about PHOENIX by watching this video.
Photo Credit: LANL

On the Inside Cover
The Los Alamos National Security Sciences Building.
Photo credit: LANL

Leadership Perspectives

LAURA STONEHILL
LDRD PROGRAM DIRECTOR

As I reflect on 2024, I feel a sense of pride and accomplishment in all that the LDRD Program has achieved this year, which is a testament to the hard work and dedication of the LDRD team.

The LDRD program plays a critical role in helping LANL meet our top strategic priorities. LDRD funding ensures that LANL can advance research and investment that addresses current and future challenges relevant to LANL missions.

Meeting current challenges requires flexibility and insight regarding the types of projects LDRD funds. In FY24, we made a significant change to our overall funding profile by expanding our Director's Initiatives (DI) portfolio. The intentional increase in both the number of DI projects funded and the amount of funding directed to the DI portfolio provides increased institutional support to Signature Institutional Commitments and other near-term priorities found within the 2024 Laboratory Agenda.

The LDRD program is funded with 5-6 percent of the Laboratory's operating budget. Projects funded by LDRD have led to prestigious awards, scientific advancements, and have produced influential scientific papers. More than half of the patents issued to LANL this year are rooted in LDRD work. Additionally, six projects with LDRD roots received 2024 R&D 100 awards, which recognize the projects as important and creative innovations in research. These outcomes are confirmation that the LDRD program yields well over its share of scientific advancements and achievements.

As I look to the future, I'm excited to see where the LDRD Program will go next. FY25 brings leadership changes to LDRD as I transition to another role at the Laboratory and Jacob Waltz takes the helm as Acting LDRD Program Director. Jacob has been with the LDRD Program for three years now as Deputy Program Director and will continue to serve the program well in his new role. It's been a privilege to be a part of this team, and I have every confidence that the program will continue to thrive and grow. I'm excited to see the important contributions that the LDRD Program will make in the years ahead.

Leadership Perspectives

JACOB WALTZ
ACTING LDRD PROGRAM DIRECTOR

The LDRD Program is a significant resource for Los Alamos National Laboratory and I can't help but be impressed by the quality and breadth of groundbreaking scientific research and discovery made possible each year through LDRD.

LDRD has made innovative contributions to every facet of national security including improvements in energy security, and advances in the Nation's ability to protect both cyber and space assets.

The U.S. Department of Energy (DOE) has charged the LDRD Programs at all DOE Laboratories with supporting high-risk, potentially high-value research. Last year the LDRD Programs at Lawrence Livermore, Los Alamos, and Sandia National Laboratories came together to release an Interlaboratory Proposal Call that provided a structured and supported path for interlaboratory collaborations on shared national strategic goals. Due to the overwhelming success of that first call, this year the collaboration was expanded to include Idaho National Laboratory, the Nevada National Security Sites, and Pacific Northwest National Laboratory. A multi-Lab call was released in July and 127 collaborative Letters of Intent were received. Following a rigorous peer review, seven projects involving multiple Laboratories were selected for funding.

The LDRD program continues to provide an important vehicle for attracting promising new staff to the Laboratory through the funding of cutting-edge research opportunities. In FY24, 65% of the Postdoctoral Researchers at the Laboratory were supported by LDRD. Additionally, 392 students worked 40 or more hours on LDRD projects. The quality of new and creative ideas these young researchers bring to the Laboratory through LDRD funded research is a significant asset to both LDRD and the Lab.

This FY24 Annual Report provides an overview of the exciting new research funded by our LDRD program. In this report you will find program highlights, impact stories, and recent accomplishments of LANL's talented research and development staff.

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Program Description

LDRD DIRECTIVES, OBJECTIVES, AND STRATEGIC CHALLENGES

Laboratory Directed Research and Development (LDRD) helps Los Alamos National Laboratory solve national security challenges through excellence in mission-focused science, technology, and engineering (ST&E). The Department of Energy (DOE) Laboratory and Site-Directed Research and Development programs are among the most impactful sources of research and development for our Nation. The heart of the LDRD program is high-risk, high-reward research that creates innovative technical solutions for some of the Nation's most difficult challenges. The LDRD programs follow strategic guidance derived from the missions of the U.S. Department of Energy, the National Nuclear Security Administration (NNSA), and the Laboratory.

To execute that strategy, the Los Alamos LDRD program creates a free market for ideas, drawing upon the creativity of the Laboratory's best and brightest researchers. The combination of strategic guidance and grassroots competition provides a continual stream of capabilities that position the Laboratory to enable agile responses to national security challenges.

Funded with five to six percent of the Laboratory's operating budget, the LDRD program makes it possible for our scientists and engineers to pursue cutting-edge research and development in support of mission. This in turn helps the Laboratory, and the Nation, maintain its position of scientific and technological leadership.

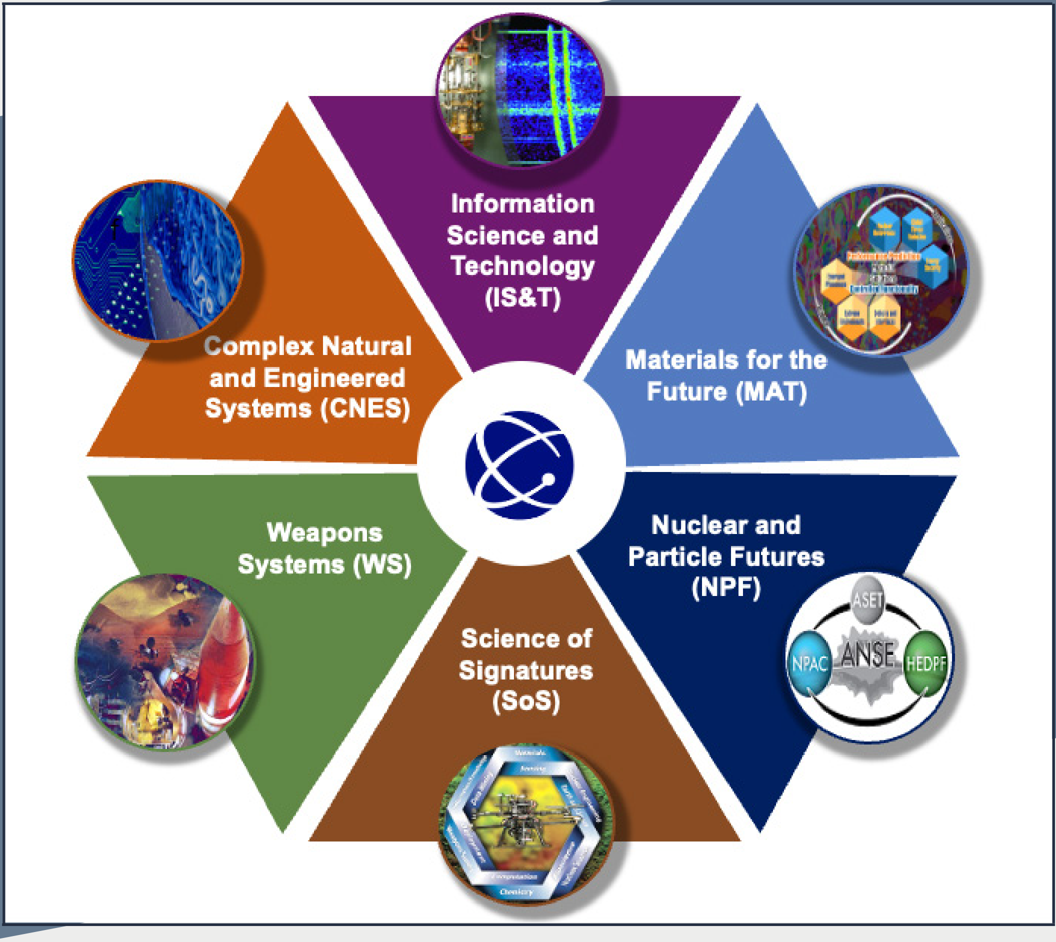
LDRD objectives guide the overall program and align with DOE Order 413.2C Chg1. The LDRD program has three objectives: Technical Vitality, Mission Agility, and Workforce Development.

The LDRD program responds to four national security challenges. This report will illustrate the Los Alamos LDRD program's successes in responding to the LDRD objectives and the national security challenges listed below:

1. *Provide an agile, flexible, and effective nuclear deterrent.*
2. *Protect against all weapons of mass destruction threats.*
3. *Deter and defend against threats in multiple domains.*
4. *Strengthen our energy and environmental national security.*

CAPABILITY PILLAR INVESTMENT

LDRD supports Laboratory strategy through our alignment with the Laboratory's Capability Pillars. These six Pillars define strategic investment areas at Los Alamos for present and future missions. All LDRD investments support one or more Capability Pillars.

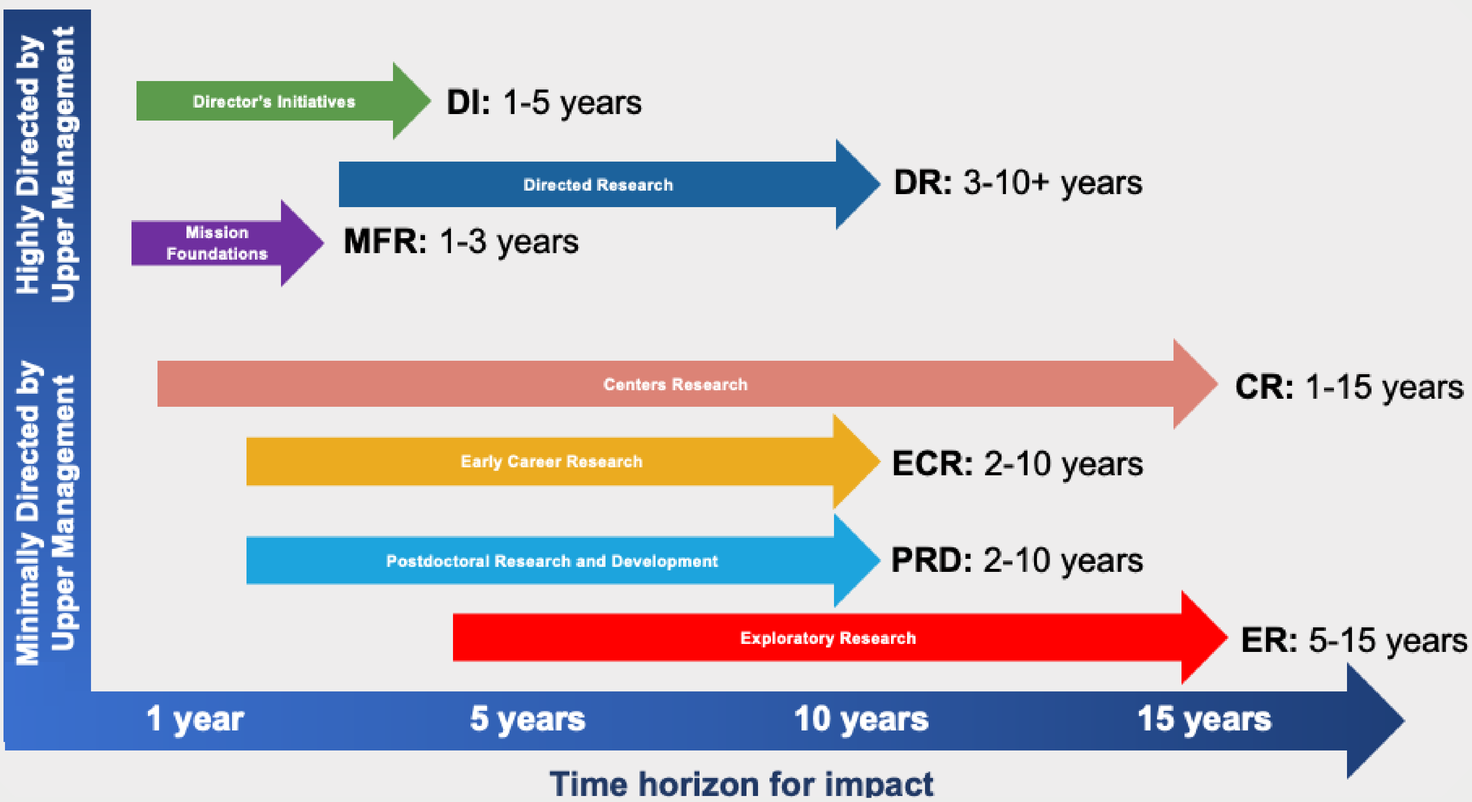


Program Structure

OVERVIEW

The Los Alamos LDRD program is organized into seven components with distinct institutional objectives:

- *Directed Research* (DR): flagship investments that create multidisciplinary solutions to complex problems defined by Lab strategy.
- *Exploratory Research* (ER): innovate at the frontiers of technical disciplines.
- *Director's Initiatives* (DI): invest in the Lab Agenda with the rigor and creativity of LDRD.
- *Mission Foundations Research* (MFR): translate discovery into novel mission solutions.
- *Early Career Research* (ECR): develop next-generation technical leaders.
- *Postdoctoral Research and Development* (PRD): attract and recruit top-quality talent into the Lab's pipeline.
- *Centers Research* (CR): incubate emerging ideas and talent in areas defined by the Lab's Strategic Centers.

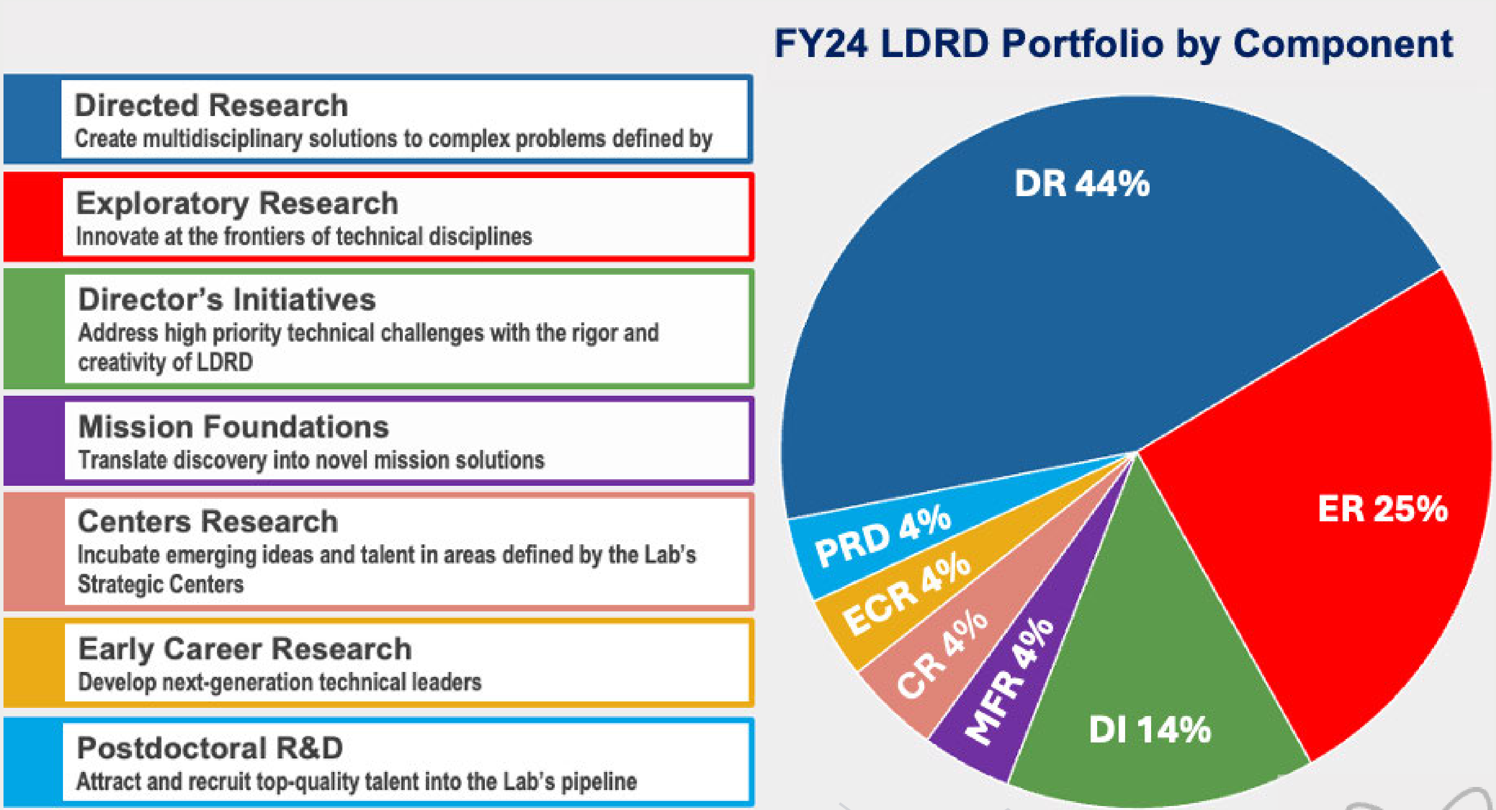


The amount of investment in each component is intentionally planned to balance the overall LDRD portfolio in both the time horizon for impact from LDRD projects and the amount of direction from Laboratory management that is involved in the selection of projects.

All seven components are discussed in further detail in this report.

In FY24, the LDRD program allocated $245M to 476 projects that incurred total costs of $233M. These projects were selected through rigorous and highly competitive peer review processes and are reviewed formally and informally throughout the fiscal year.

Funds were intentionally distributed across the seven LDRD components. The graphic below shows the percentage of the total FY24 LDRD budget invested in each of the seven components.

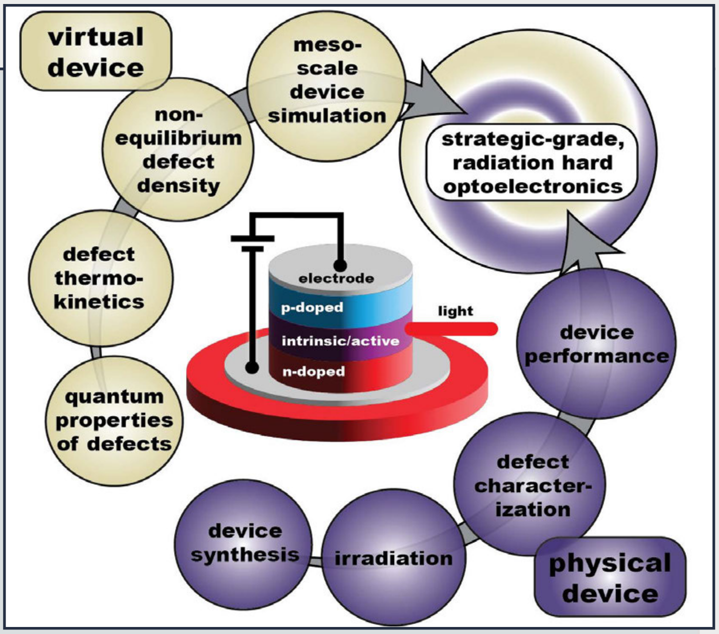


DIRECTED RESEARCH: CREATE MULTIDISCIPLINARY SOLUTIONS TO COMPLEX PROBLEMS DEFINED BY LABORATORY STRATEGY

In FY24, LDRD funded 59 Directed Research (DR) projects, investing $103.6M, which represents 44% of the program's research funds.

DR projects are aligned to key competency or technology-development areas vital to LDRD's long-term ability to enable the Lab to execute its missions. Funding for individual DR projects is approximately $2M per year for three years.

The annual planning for DR directly ties to the Laboratory's Capability Pillars. This planning is communicated through the Strategic Investment Plan (SIP) which is published annually. Laboratory leadership provides strategic guidance to SIP Development Teams associated with each Pillar. The teams then engage with Laboratory staff to identify investment priorities for the upcoming fiscal year that are consistent with and supportive of the long-term Pillar strategy. Priorities may include not just strategic capabilities, but also mission challenges requiring new and innovative approaches.



Directed Research in Action

Optoelectronic systems, such as laser diodes, are poised to play a crucial role in the United States. However, for these systems to be viable, it is critical to understand and mitigate the damaging effects of ionizing radiation. While these components are readily available, off-the-shelf commercial systems, they are extremely challenging to study due to both the inherent complexity of these systems as well as the proprietary nature of the composition. These considerations make understanding the fundamental interaction between ionizing radiation and device performance essentially impossible.

The goal of this project is to simplify the problem by making, measuring, and modeling a simplified, yet functional, laser system with the ultimate goal of developing the capability to predict the performance of semiconductor injection lasers upon exposure to radiation and to enable the development of radiation-hard optoelectronic devices.

PI: Blas Uberuaga
LDRD project: 20240033DR M3ONARCH: Making, Measuring, and Modeling Optoelectronics for Next-generation Applied Radiation-hard Components and Hardware

EXPLORATORY RESEARCH: INNOVATE AT THE FRONTIERS OF TECHNICAL DISCIPLINES

In FY24, LDRD funded 201 Exploratory Research (ER) projects, investing $59.2M which represents 25% of the program's research funds.

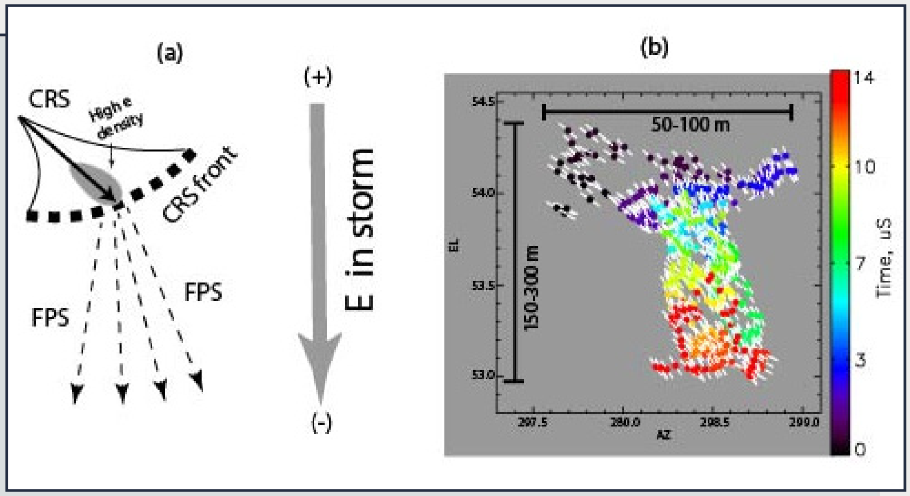
The ER component is the most important channel for purely bottom-up creativity at the Laboratory. Initiated by technical staff from across the Laboratory, ER projects explore highly innovative ideas in 10 Technical Categories that underpin Laboratory missions. Funding for individual ER projects is approximately $350K per year for three years.

Exploratory Research also funds ER Seedlings and ER Interlaboratory projects. ER Seedlings projects are funded for 12 months at approximately $150K per project and are intended to address the most untested, high-risk aspects of a new idea. Interlaboratory projects are funded for two and a half years and offer a structured and supported path for multi-Laboratory collaborations on key shared national strategic goals. Funding levels vary for Interlaboratory projects.

Exploratory Research in Action

Lightning is a fundamental background in the Nation's nuclear detonation detection missions. Understanding its signatures is critically important for reliable detonation identification. This project supports directly the current nuclear detection missions.

The project is focused on understanding the fundamental physics of lightning initiation with unique and advanced 3-dimensional radio frequency source mapping, polarization measurement, and radiation beam-pattern reconstruction, together with an array of gamma-ray detectors. In addition to the main research goal, a number of new understandings of other lightning discharge processes are envisioned.



Left: The project's lightning initiation concept. A cosmic-ray shower enters the cloud and produces thermal electrons behind its front around the core (gray oval). This region with a sharp front enhances field ahead of the front and produces downward positive streamers in the downward E-field. Right: 2D angular (az vs el) observation of initial 14 microseconds for an IC. Colored dots are mapped sources that start from upper-left (black) and move toward lower-right (blue) in first 2 microseconds Thereafter, sources move mostly vertically downward (light blue to red). White bars are polarization orientations. Credit: LANL

The results of this project will have a substantial impact on the Nation's next generation nuclear detection missions, especially on the space-based nuclear electromagnetic pulse (EMP) detection.

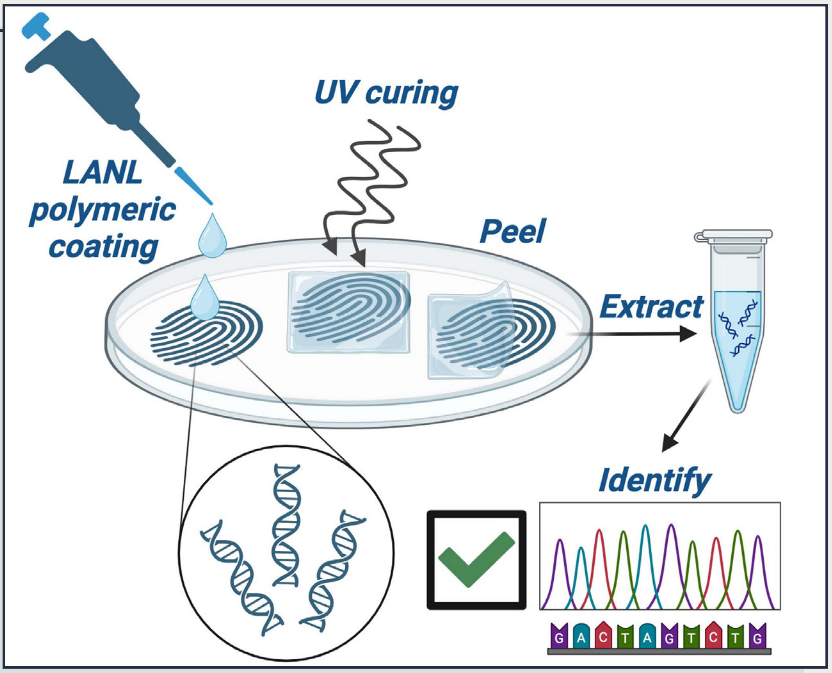
PI: Xuan-Min Shao
LDRD Project 20230223ER the Genesis of Lightning Flash

Exploratory Research Seedlings in Action

Touch DNA (Deoxyribonucleic Acid) evidence is becoming increasingly relevant for forensic applications, but due to limitations in collection techniques the approach is still highly speculative and unreliable for standard investigations.

The primary goal of this Seedlings project led by researcher Ann Junghans is to understand and improve DNA (Deoxyribonucleic Acid) removal, both in terms of quantity and quality, as compared to traditional techniques. If successful, this work could make it possible to identify an individual by the DNA (Deoxyribonucleic Acid) left in a single fingerprint.

PI: Ann Junghans
LDRD Project: 20240794ER Collecting Touch DNA- A Fingerprint is all it takes



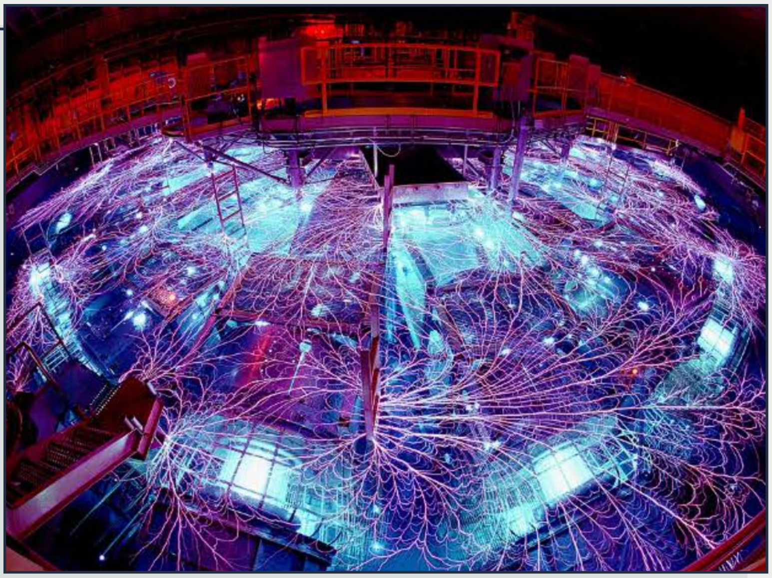
LANL-developed curable gel coatings will be used to demonstrate a new method to improve reliability of touch DNA collection. The curable gel coatings will enable access to previously difficult-to-sample surfaces, improvements in DNA collection efficiency, and preservation of the DNA sample integrity.

Interlaboratory Research in Action

This collaborative, multi-lab project involving Los Alamos, Lawrence Livermore, and Sandia National Laboratories is using tensor network discretizations to enable next-generation simulation capabilities on next-generation supercomputing architectures to enable robust predictive capabilities for next-generation pulsed power high energy density science.

The overarching goals of the project are to address the deficiencies of current pulsed power modeling capabilities by significantly increasing the model and simulation fidelity and extensibility available to designers.

LANL PI: Boian Alexandrov
LLNL PI: Pierson Guthrey
Sandia PI: Nathan Roberts
Project: 20240705ER Predictive Ultrafast Low-Rank Simulations via Embedded Tensor Networks



The integration of the unique expertise of LANL, SNL and LLNL in SmartTensors AI, Plasma Physics Modeling & Simulation and Pulsed Power, and High Performance Computing will lead to a revolutionary new capability to directly simulate plasma kinetics and corresponding generation of electromagnetic fields. Power flow designers at LLNL and Z-pinch designers at SNL have indicated that this solver technology would benefit from having this new tool available to them.
Image: Sandia's Z machine. [Photo by Randy Montoya]

DIRECTOR'S INITIATIVE: INVEST IN THE LABORATORY AGENDA WITH THE RIGOR AND CREATIVITY OF LDRD

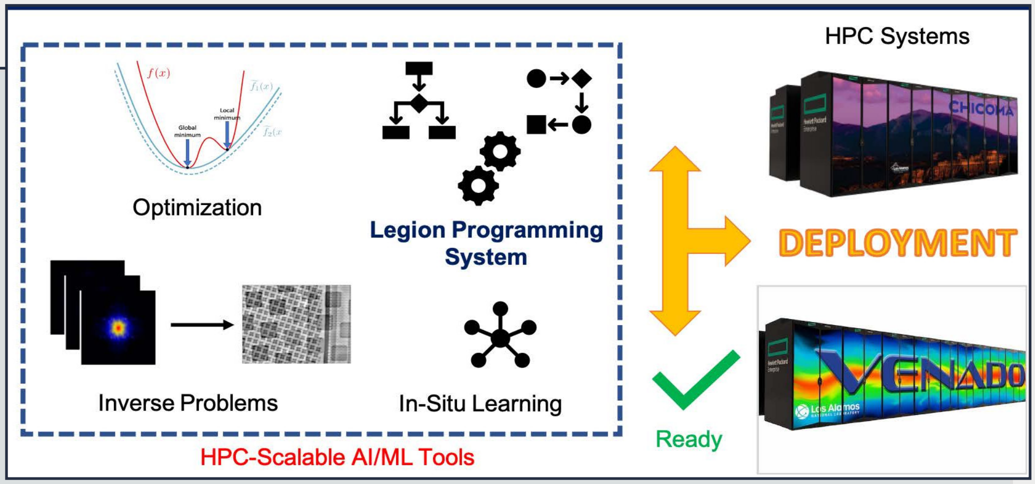
In FY24, LDRD funded 28 Director's Initiative (DI) projects, investing $32.8M which represents 14% of the program's research funds.

LDRD DI projects tie directly to Signature Institutional Commitments and critical outcomes within the Laboratory Agenda. The senior Laboratory leaders (typically Associate Laboratory Directors) responsible for the Laboratory Agenda work with the LDRD Program Office and the Deputy Director for Science, Technology, and Engineering to identify strategic growth areas and potential projects. Proposals are held to the same standards of peer review as other LDRD investment components.

Associate Laboratory Directors (ALDs) typically begin planning before the start of the FY, communicating their project priorities to the LDRD Program Office. The LDRD Office follows with requests for individual proposals and peer review. Most initiatives for the year are in place by January. The duration of Director's Initiatives is between nine months and three years.

Director's Initiative Research in Action

High performance computing (HPC) has the potential of being an unprecedented resource for AI/ML at DOE. This includes the ability to generate huge amounts of training data using traditional modeling and simulation.



This project focused on developing HPC-scalable AI/ML tools targeting two specific AI/ML science building blocks, optimization and inverse problems, enabled by two crosscutting technologies, in-situ learning workflows and the Legion Programming System, and will enable support future large scale demonstrations of AI/ML enhanced capabilities using LANL's new supercomputer Venado.

This project focused on the development and demonstration of Artificial Intelligence (AI) and Machine Learning (ML) tools that specifically scale to current and future LANL High Performance Computing (HPC) systems. The tools are necessary for enabling computational breakthroughs critical to advance a diverse range of problems in the space of Los Alamos National Laboratory's missions in science, energy, and security. The project was able to successfully advancing software tools and contributed to a more efficient algorithmic exploration, allowing the ability to dedicate more time to improving methods and less time tuning to particular hardware resources.

PI: Aric Hagberg
LDRD Project: 20230771DI High-Performance Artificial Intelligence

MISSION FOUNDATIONS RESEARCH: TRANSLATE DISCOVERY INTO NOVEL MISSION SOLUTIONS

In FY24, LDRD funded 28 Mission Foundations Research (MFR) projects, investing $9.5M which represents 4% of the program's research funds.

MFR is an intentional investment in applied science and engineering relevant to national security missions and addresses mission needs in the technology readiness level (TRL) 3-5 regime. Proposals must respond to "mission problem statements" reflective of mission needs across the Laboratory and are subject to rigorous peer review that assesses alignment with the LDRD program objectives– Technical Vitality, Mission Agility, and Workforce Development. Individual projects are funded at $500K - $665K per year, with projects running 1-2 years in length.

Mission Foundations Research in Action

Researcher Michael Pettes recently led an MFR project that was focused on solving big data characterization methods to make the use of fast electron detectors more practical.

Pettes and his team developed an uncertainty-based four-dimensional scanning transmission electron microscopy (4D STEM) capability. This capability allows for real-time data analyses of crystallographic orientation and strain at the nanoscale to thereby understand key fundamental science questions in actinide research.

The team further enhanced the technology by adding a new multi-beam electron diffraction capability to enable three-dimensional nanoscale characterization of crystal orientation and strain, a first of its kind.

Read more about the work that Pettes and his team have accomplished through their 4D STEM research in this recent cover article.

PI: Michael Pettes
LDRD Project: 20220485MFR Coupling Multiple Patterned Electron Probes for Real Time Orientation, Lattice Parameter, and Strain Mapping at the Nanoscale

Additional LDRD projects that contributed to the ACS NANO article:

- *20230014DR Discovering Quantum Anomalies Through Strain (PI: Michael Pettes)*
- *20190516ECR Electronic Transport in Atomically Thin Materials at Far from Mechanical Equilibrium Conditions (PI: Michael Pettes)*

EARLY CAREER RESEARCH: DEVELOP NEXT-GENERATION TECHNICAL LEADERS

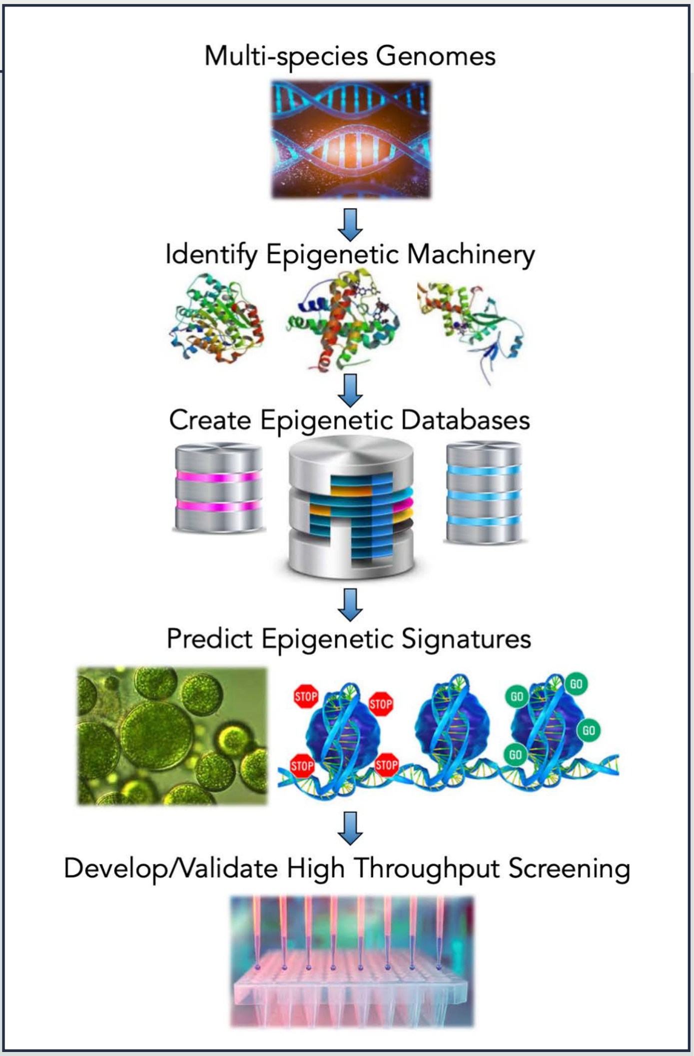
In FY24, LDRD funded 53 Early Career Research (ECR) projects, investing $8.6M, which represents 4% of the program's research funds.

The ECR component of the LDRD program is designed to strengthen the Laboratory's scientific workforce by providing support to exceptional staff members during their crucial early career years. The intent is to support the development of early career researchers, aiding in the transition from postdoc or student to full-time staff member, and to stimulate research in disciplines supported by the LDRD program. ECR projects are individually funded up to $240K per year for two years. Early Career Research PIs must have received their highest degree within the last ten years and been hired as a Laboratory technical staff member no more than three years prior to the call.

Early Career Research in Action

Epigenetic processes are the gatekeepers of the genome: they control the accessibility of genetic information and how a cell responds to its environment. Research has shown that epigenetic processes play a significant role in disease progression, including cancer and mental health disorders. If one can control epigenetic processes in an organism, one can control the behavior of the organism, including its physiology.

Researcher Christina Steadman led an ECR project that created a combinatorial toolkit for epigenetic manipulation of behavior. The project team built a novel computational pipeline and software package to predict epigenetic processes in microalgae. Predictions were validated via high-throughput screening (HTS) assays we developed for DNA methylation (using Nanopore sequencing) and histone modifications (using high-resolution mass spectrometry). The team was then able to successfully manipulate epigenetic processes in microalgae.



PI: Christina Steadman
LDRD Project: 20220621ECR Prediction and Manipulation of Epigenetic Processes for Enhanced Behavior

POSTDOCTORAL RESEARCH AND DEVELOPMENT: ATTRACT AND RECRUIT TOP-QUALITY TALENT INTO THE LAB'S PIPELINE

In FY24, LDRD funded 97 Postdoctoral Research and Development (PRD) projects, investing $8.9M, which represents 4% of the program's research funds.

The PRD component of the LDRD program ensures the vitality of the Laboratory by recruiting early career researchers. Through this component, LDRD funds Postdoctoral Fellows to work under the mentorship of PIs on highly innovative projects. Postdoctoral projects are individually funded up to $200K per year for 2-3 years. The review and selection processes are conducted under by the Los Alamos National Laboratory Postdoc Program Office.

PRD projects are funded under two appointment types:

- Director's Postdoctoral Fellows - Funding for this appointment type follows a stepped approach: 100% (year 1), 66% (year 2), and 33% (year 3, if the project is extended for a third year). The intent is to encourage the Fellow to engage in programmatic work as their postdoctoral appointment progresses. This familiarity often leads to long-term Lab career opportunities.
- Distinguished Postdoctoral Fellows- These PRD Fellows receive full-time support at a highly competitive salary for three years. Full-time support allows the Distinguished Fellows considerable freedom to pursue their own ideas.

Postdoctoral Research in Action

Researchers Mark Zammit and Isuru Ariyarathna are leading a project that is focused on opacity calculations of small molecules as well as performing highly accurate multi-reference quantum chemistry calculations of iron hydride (FeH) and other molecules of importance.

Ariyarthna recently shared some of the recent findings from this work in this cover article that explores the use of experimental spectroscopic studies and computational explorations to gain insight into the electronic structures of molecules and predicting their reactivities.

PI: Mark Zammit
Postdoctoral Researcher: Isuru Ariyarathna
LDRD project: 20240737PRD1 Development of Molecular Opacities and Beyond

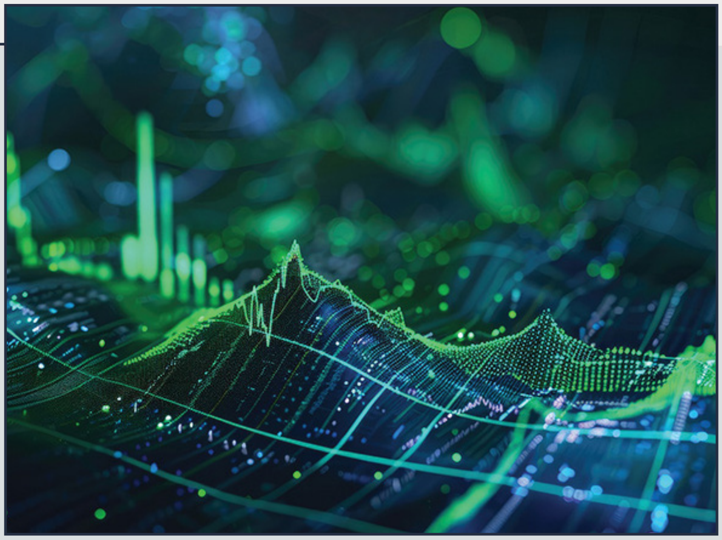
CENTERS RESEARCH: INCUBATE EMERGING IDEAS AND TALENT IN AREAS DEFINED BY THE LAB'S STRATEGIC CENTERS

In FY24, LDRD funded 10 Centers Research (CR) projects, investing $10.1M, which represents 4% of the program's research funds.

To infuse new ideas and people into the Laboratory, LDRD has made a commitment to partner with the Lab's "Strategic Centers." The CR component is focused on developing the Nation's next-generation workforce and leadership talent and serving as an incubator for the introduction of emerging science, technology, and engineering (ST&E) into Laboratory missions. CR projects are typically funded up to three years and single-year per project funding ranges from approximately $500K-$1,900K.

Centers Research in Action

Quantum computers are still a nascent technology, but researchers are busy building complex machine learning algorithms to test the capabilities of quantum learning. Sometimes, however, their algorithms hit a mysterious dead end; a mathematical path from which there is no way forward or backward — the dreaded barren plateau.



Barren plateaus were a little-understood but common problem in quantum algorithm development. Credit: LANL

Barren plateaus were a little-understood but common problem in quantum algorithm development. Sometimes, after months of work, researchers would run their algorithm and it would unexpectedly fail. Scientists had developed theories as to why barren plateaus exist and had even adopted sets of practices to avoid them. But no one knew the underlying cause of this mathematical equivalent of a dead end.

Los Alamos researchers developed an equation that was able to predict barren plateaus in any quantum optimization algorithm. Even more, their equation uncovered new sources of barren plateaus. What the researchers discovered is that specialization, rather than generalization, is the key to avoiding barren plateaus. This breakthrough allows scientists to understand and unify all known sources of barren plateaus, and thus avoid them as they build their algorithms.

This research represents the first time anyone has successfully developed a unified, mathematical approach to identifying barren plateaus. The results will have a far-reaching impact in the field of quantum computing, which has rapidly developed in recent years.

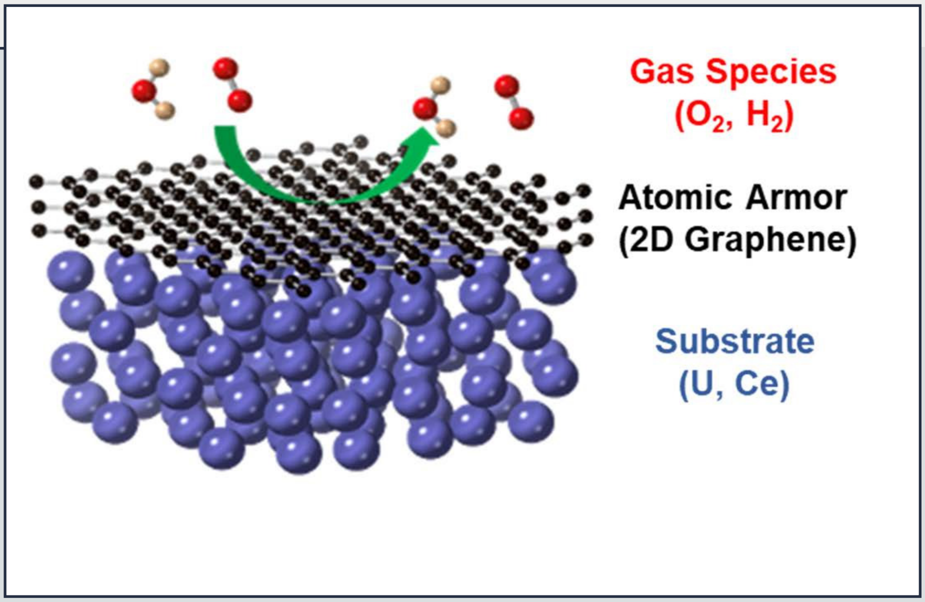
This work was led in part by Martin Larocca on LDRD Center's project 20220546CR and by researcher Marco Cerezo on LDRD projects 20230049DR and 20230527ECR. Read more about this breakthrough here.

RESERVE FUNDING

Not all of the LDRD budget is allocated to individual projects at the beginning of the fiscal year. The LDRD program employs Reserve funding for strategic initiatives to facilitate institutional agility when addressing time-urgent, national security challenges.

When investing these Reserve funds, LDRD will typically turn to the Associate Laboratory Directors for guidance and priorities. Reserve proposals are held to the same peer review standards as the annual calls. During FY24, a total of $3.5M in Reserve funds were invested, with some funds added to existing projects and the remainder used to start new projects during the year. A total of eight projects received Reserve funding in FY24.

Reserve Funding in Action



Schematic representation of the project's innovative 2D material coating to protect reactive and radioactive substrates from corrosive species.

The corrosion of reactive metals, including uranium, is a persistent problem for their safe handling, reliable usage, and long-term storage. Since the corrosion starts near material surfaces, coating them with impermeable, chemically inert, thermodynamically stable, and atomically thin two-dimensional (2D) materials, such as graphene, can be a promising robust approach to prevent environmental degradation, without compromising their nuclear performance. However, radiation damage effects on structural integrity of the 2D coating impose a unique challenge to actinides due to their persistent self-irradiation. Potential corrosion-irradiation synergy may further impact the long-term efficacy of the 2D coating protection applied to actinide surfaces.

This project led by researcher Yongqiang Wang resulted in successful demonstrations of the anti-corrosion performance of 2D coating technology on depleted uranium against corrosive gas and its tolerance to self-irradiation damage in decadal time scale. The results position LANL as the pioneer and leader in applying state-of-the-art material and technology in improving the reliability and reducing the cost in stockpile stewardship.

PI: Yongqiang Wang
LDRD Project: 20240473DR Two-Dimensional (2D) Graphene as Corrosion Protection Barrier for Uranium

Program Value

Congress established the LDRD program at the DOE National Laboratories in 1991 to foster excellence in ST&E and to ensure the Laboratories are technically vital and prepared to meet today's needs and tomorrow's challenges.

LDRD supports high-risk, potentially high-payoff research and development, serving as a key resource for addressing the ST&E goals of the Laboratory. Through careful investment of LDRD funds, the Laboratory builds its reputation, recruits and retains excellent scientists and engineers, and prepares to meet evolving national needs.

The metrics shared on the following pages demonstrate how the LDRD program at Los Alamos successfully addresses the LDRD program objectives of Technical Vitality, Mission Agility, and Workforce Development.

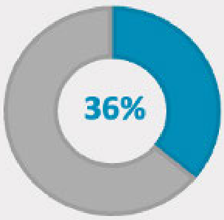
FY24 KEY PERFORMANCE INDICATORS

$233M
Total LDRD Program Cost (5.72% of LDRD-eligible LANL budget)

476
Total Number of LDRD Projects

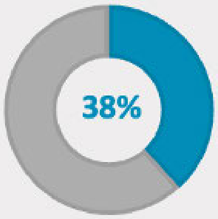
193
New LDRD Projects in 2024

Publications



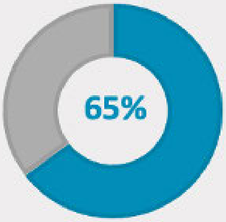
705 of 1938 unclassified publications at LANL can be attributed to LDRD

Publication Citations



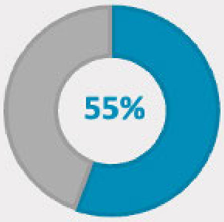
2016 of 5254 citations of unclassified publications at LANL can be attributed to LDRD

Postdocs



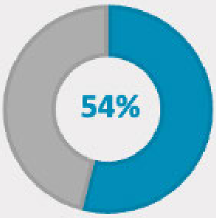
471 of 728 Postdocs at LANL were supported by LDRD

Postdoc Conversions



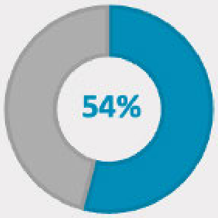
56 of 101 Postdoc conversions at LANL involved LDRD supported Postdocs

Patents



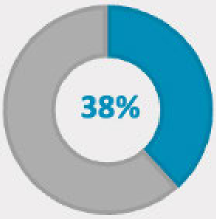
14 of 26 U.S. patents issued at LANL can be attributed to LDRD

Invention Disclosures



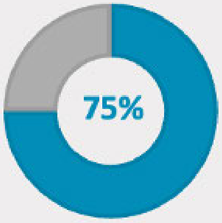
40 of 74 invention disclosures issued at LANL can be attributed to LDRD

Software Copyrights



52 of 136 U.S. software copyrights issued at LANL can be attributed to LDRD

R&D 100 Awards



6 of 9 R&D 100 Awards at LANL can be attributed to LDRD

Performance Indicators: LDRD at Los Alamos National Laboratory

This section presents both short and long-term performance indicators that LDRD maintains to evaluate the success of LDRD projects. LDRD yields well over its share of intellectual property, postdoc conversions, publications, patents, and technical awards.

INTELLECTUAL PROPERTY

LDRD funds cutting-edge research that has a large impact on the Laboratory's intellectual property. LDRD projects lead to a disproportionately large percentage of the patents and copyrights issued for Los Alamos research.

US Patents

Number of US patents issued in a given FY.
LDRD supported: Patents issued that would not exist if not for initial work funded by LDRD.

	FY20	FY21	FY22	FY23	FY24
LANL U.S. Patents	46	46	38	30	14
LDRD Supported	19	14	19	14	26
% Due to LDRD	41%	30%	50%	47%	54%

Software Copyrights

Number of software copyrights created in a given FY.
LDRD Supported: Copyrights issued that would not exist if not for initial work funded by LDRD.

	FY20	FY21	FY22	FY23	FY24
LANL Software Copyrights	119	120	115	118	136
LDRD Supported	39	48	47	54	52
% Due to LDRD	33%	40%	41%	46%	38%

Invention Disclosures

Number of declarations and initial records of an invention (a new device, method, or process developed from study and experimentation).
LDRD Supported: Disclosures issued that would not exist if not for initial work funded by LDRD.

	FY20	FY21	FY22	FY23	FY24
LANL Disclosures	115	101	73	72	74
LDRD Supported	34	33	30	26	40
% Due to LDRD	30%	33%	41%	36%	54%

PEER-REVIEWED PUBLICATIONS

Technical Vitality

The large volume of high-quality peer-reviewed publications produced through LDRD funded work help the Laboratory maintain a strong presence and scientific reputation in the broader scientific community.

Publications

Number of peer-reviewed publications.
LDRD supported: Publications for which LDRD made a substantial contribution.

	FY20	FY21	FY22	FY23	FY24
LANL Publications	1,971	2,207	1,929	2,090	1,938
LDRD Supported	678	830	796	755	705
% Due to LDRD	34%	38%	41%	36%	36%

Citations

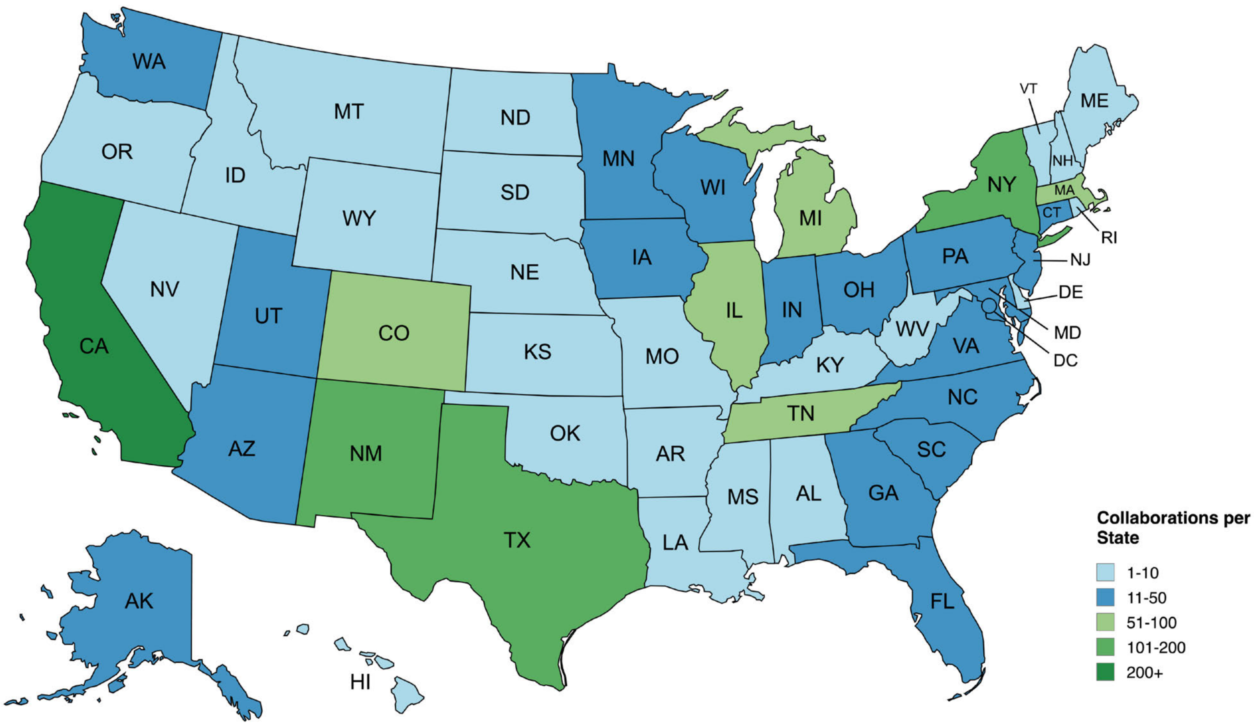
Number of times a peer review publication has been cited since the publication year.
LDRD Supported: Citations of publications for which LDRD made a substantial contribution.

Publication Year	FY20	FY21	FY22	FY23	FY24
LANL Citations	92855	42011	28997	15,926	5253
LDRD Supported	41915	18338	12199	6999	2016
% Due to LDRD	45%	45%	42%	44%	38%

BROAD INTELLECTUAL ENGAGEMENT

External collaborations are an essential part of the research and development in LDRD. By working with other national laboratories, academia, and industry, LDRD investigators engage with experts across the Nation and around the world. Most external collaborations under LDRD are on a no-exchange-of-funds basis- collaborators use their own funding for the mutual benefit of working together and promoting scientific/ engineering discovery.

In FY23 and FY24 LDRD researchers reported 2,019 external collaborations, including 1,623 collaborations with US scientists and engineers and 396 with foreign collaborators.



Collaborations within the United States (U.S.) took place in all 50 states. California had the highest number of reported collaborations at 289, as shown in the map above.

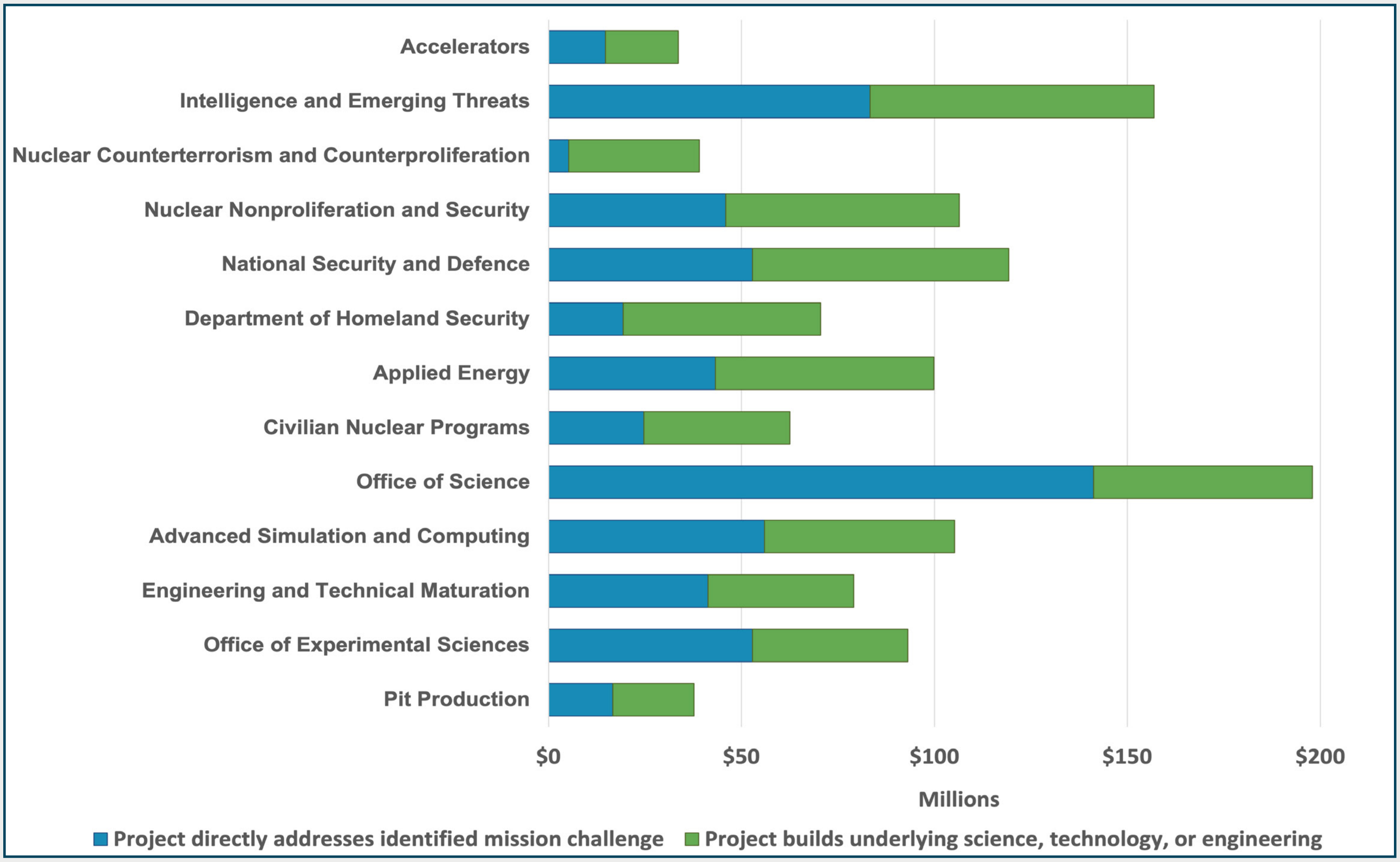
U.S. collaborations were reported with 317 different organizations. The graph to the right shows which U.S. organizations had more than 25 reported collaborations with LDRD researchers.

MISSION RELEVANCE

Mission Agility

Mission relevance is one of the most important criteria in the evaluation of the LDRD program, as well as a potential LDRD project. It is carefully considered in project selection and tracked annually through the data sheet process. Many of the technologies that put Los Alamos on the map have deep roots in LDRD and are valuable to DOE and NNSA mission areas of nuclear security, energy security, environmental remediation, and scientific discovery and innovation. LDRD work also benefits the national security missions of the Department of Homeland Security, the Department of Defense, and other Federal agencies. As a result, the ST&E innovations from LDRD provide multiple benefits to all Los Alamos stakeholders, consistent with Congressional intent and the Laboratory's technical strategy.

Mission Impact of the FY24 LDRD Portfolio ($M)



Los Alamos LDRD projects are required to address one or more mission areas. Investment in one project often contributes to and impacts multiple missions. The result is that the sum of the total LDRD investment in the relevant mission impact areas shown in the chart above is far greater than the annual LDRD budget.

Workforce Development

SCIENCE AND ENGINEERING TALENT PIPELINE

The innovative research and development that LDRD provides is an important vehicle for recruiting the brightest researchers to Los Alamos National Laboratory, where they become technical innovators and leaders. LDRD is also instrumental in retaining new talent from the student and postdoc pool at the Laboratory.

Postdoctoral Researcher Support

Number of postdoctoral researchers working full- or part-time for the Laboratory.
LDRD supported: Postdoctoral researchers charging at least 10% of their time to LDRD.

	FY20	FY21	FY22	FY23	FY24
LANL Postdocs	655	665	652	656	728
LDRD Supported	363	391	389	402	471
% Due to LDRD	55%	59%	60%	61%	65%

Postdoctoral Researcher Conversions

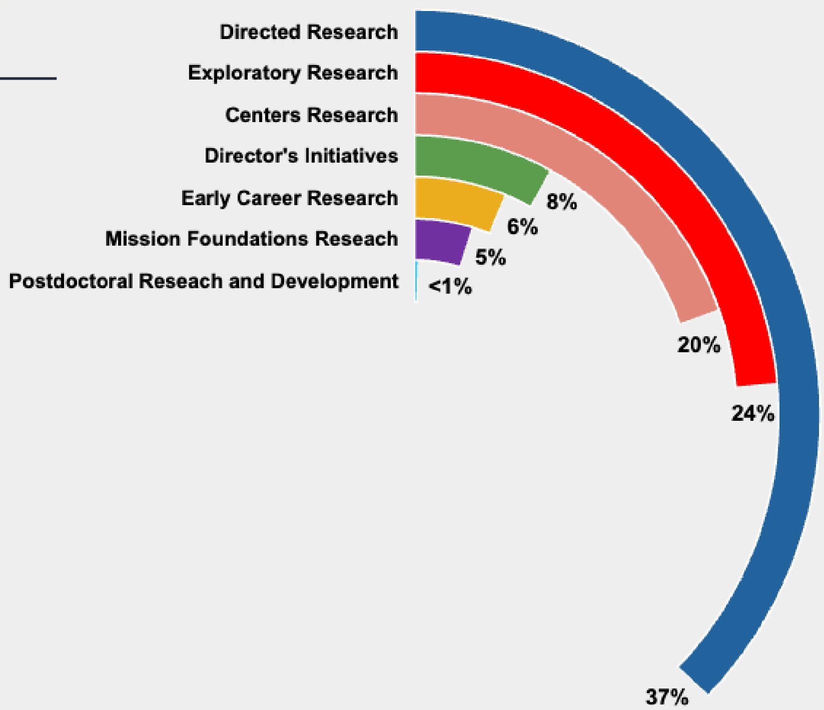
Number of conversions from postdoctoral researcher to a member of the staff.
LDRD Supported: Conversion of postdoctoral researchers who charged at least 10% of their time to LDRD in FY23.

	FY20	FY21	FY22	FY23	FY24
LANL Conversions	75	81	120	93	101
LDRD Supported	35	44	58	51	56
% Due to LDRD	47%	54%	48%	55%	55%

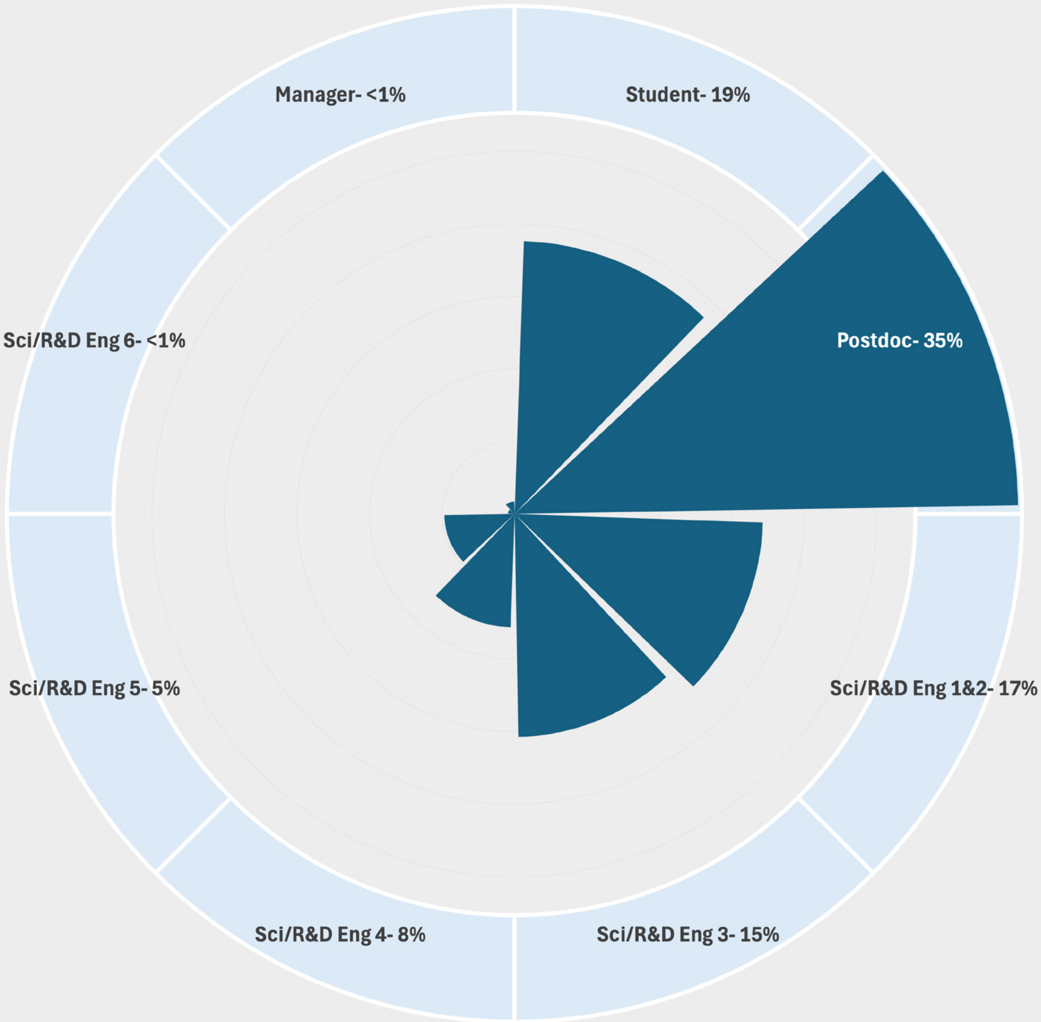
Students Supported by LDRD

There are many opportunities for students to play important supporting roles on LDRD projects. For example, a student might work with an early career staff member on a project, where the early career staff member would serve as the PI and the student would serve a significant secondary role to that PI. LDRD is supportive of students working in a Co-Investigator role on any LDRD project.

In FY24, 392 students worked at least 40 hours on LDRD projects. The graph to the right provides a breakdown, by component, of the total student hours charged to LDRD in FY24 for those students who worked 40 or more hours on LDRD projects.



Workforce Development



LDRD Invests in Early Career Staff

LDRD plays in important role in attracting, developing, and retaining an exceptionally talented and creative workforce who are able to address some of our Nation's most difficult challenges. The graph above illustrates the large engagement of early career staff, postdocs, and students in the LDRD program. The graph shows a breakdown of the total hours charged to LDRD in FY24 by students, postdoctoral students, scientists, research and development (R&D) engineers, and managers. As shown, 19% of the total labor hours charged to LDRD were charged by students, 35% of the total were charged by postdoctoral researchers, and 17% of the total were charged by Scientists/R&D Engineers 1 & 2. It is not uncommon for managers to continue contributing important R&D to a research project; in FY24, slightly less than 1% of the total time charged was charged by managers working on LDRD projects.

EARLY CAREER SPOTLIGHTS

Workforce Development

Keegan Kelly and Dan O'Malley

Two LDRD Researchers win DOE Early Career Research Program Awards

Keegan Kelly of the Physics division, and Daniel O'Malley of the Earth and Environmental Sciences division, each won a DOE Early Career Research Program award, which provides five years of funding for an R&D project relevant to an Office of Science program area of importance to basic energy sciences.

Keegan, who has led two LDRD projects, including an FY19 LDRD Early Career Research project, will be leading a DOE project that is focused on developing a new capability to better measure nuclear data of importance to fusion reactors and other areas of nuclear physics.

Dan, who has led four LDRD projects, including an FY14 Postdoctoral project and an FY20 Early Career Research project, will be leading a DOE project that is using quantum computing and machine learning to represent a wider range of scales in complex fracture networks of importance to basic energy sciences. "Having two of our premier early-career researchers selected for this prestigious award is a great honor, both for the Laboratory and for the awardees themselves," said Laboratory Director Thom Mason. "Congratulations to both Keegan and Dan for distinguishing themselves in their respective fields. I look forward to seeing the outcomes of their projects."

LDRD Postdoctoral Researcher earns Outstanding Postdoc Award

Isuru Ariyarathna, a LDRD Richard Feynman Distinguished Postdoctoral Fellow who works with the Laboratory's Theoretical division, has earned a Wiley Computers in Chemistry Outstanding Postdoc Award. The program is organized by the American Chemical Society's Computers in Chemistry Division (or COMP).

Ariyarathna was recognized for his research focused on "How to design hyperreactive superalkalis: lessons learned from wavefunction theory and density functional theory."

Ariyarathna's current research spans four main directions of chemical discoveries: studying "superatoms" and the materials they form, conducting molecular encapsulation for pharmaceutical/medicinal and material science applications, designing bottom-up industrial-grade catalysts and working in spectroscopy research. To date, Ariyarathna has disseminated work through 42 refereed journal articles. He holds a doctorate in theoretical chemistry from Auburn University.

The Long-term Impacts of LDRD Investments

The LDRD program is an investment in the Nation's future, ensuring mission support that is often realized after many years. This section highlights the longer-term (>5 year) impact of LDRD as a national asset. These performance indicators will be updated annually. As it is expected that the data may vary from year to year, long-term running totals will also be included and updated every five years.

Background

As part of a commitment to continuous improvement, representatives from each LDRD program at the NNSA Laboratories regularly participate in a working group to share best practices and discuss strategies for tracking the long-term impact of LDRD investments. In FY20, the working group finalized a combination of common quantitative and qualitative long-term indicators, emphasizing a systematic approach. Additionally, the working group recognized that the individual Laboratories may choose to report other long-term indicators that fit their unique missions and capabilities.

Alignment with LDRD Objectives

The collective selection of indicators (both numerical and qualitative) illustrate the long-term payoffs and success of LDRD, with respect to all three LDRD objectives (Technical Vitality, Mission Agility, Workforce Development). Because indicators crosscut objectives, there is not an intent to provide a 1:1 mapping of indicators with objectives.

Importance of Qualitative Data

The difficulty of developing numerical indicators for success in R&D programs is widely recognized. The metrics working group was able to develop numerical success indicators for both Technical Vitality and Workforce Development. "Success stories" were found to be more flexible to capture the successes in Mission Agility, as well as aspects of the other two LDRD objectives that are not well-captured by numerical metrics.

Tracing Impact Back to LDRD

Throughout this section, you will see references to "LDRD roots." There is often a lot of discussion with PIs about what it means for an accomplishment to have "LDRD roots." A simple case would be if an idea for an invention arises during an LDRD project and work on the invention is completed during the period of LDRD investment. But R&D often does not advance on such a short timescale. In general, an accomplishment (invention, paper, capability, etc.) is determined to have LDRD roots if there are one or more LDRD projects without which the accomplishment would never have come into being. In other words, if one can identify an LDRD project that was critical to the accomplishment, then it is considered to have "roots" in that LDRD project. Other relevant definitions for the metrics shared are included in the sections to follow.

SCIENCE AND ENGINEERING TALENT PIPELINE

Workforce Development

Professional Fellows (American Physical Society)

One relevant indicator of advancement and leadership in an ST&E field is the election of individuals as Fellows of professional societies. This indicator reflects success for both the individual researcher and the Laboratory as a whole. APS Fellowship is awarded based on scientific merit and impact over an extended period of time. (In contrast, some professional societies may also award Fellow status based on service to the society.) Over the past 10 years, 86% of Los Alamos National Laboratory's (LANL) APS Fellows have had LDRD experience.

LDRD and American Physical Society Fellows at Los Alamos National Laboratory

	Single-Year Statistics			Five Years		Ten Years
	FY22	FY23	FY24	FY15-FY19	FY20-FY24	FY15-FY24
Total Awards	3	1	2	34	15	49
Awards with LDRD Roots	2	1	2	30	12	42
% with LDRD Roots	67%	100%	100%	88%	80%	86%
Average Years from First LDRD Experience	14	10	25	11.6	15	12.5

Two LANL Researchers Elected 2024 APS Fellow have LDRD Experience

Tanmoy Bhattacharya *was named an APS Fellow for his groundbreaking contributions to computational and fundamental physics, especially to lattice QCD and computational biology, including computations of the QCD equation of state at finite temperature, the neutron electric dipole moment, and the timing of the spread of the modern HIV pandemic. Bhattacharya is the author of more than 150 peer-reviewed publications. His current physics work is focused on using supercomputers to simulate quantum field theory to explore new physics, employing machine learning to drive physics calculations, and investigating the impact of quantum computing on quantum field theory. Bhattacharya's work in LDRD first began in 1986 as the PI on an Exploratory Research project.*

Stefano Gandolfi *was named an APS Fellow for his work developing advanced Quantum Monte Carlo methods in nuclear physics, enabling a simultaneous understanding of nuclei and dense neutron star matter that has strengthened connections across nuclear physics and nuclear astrophysics. Gandolfi's work has centered on challenging problems in nuclear physics and nuclear astrophysics, including the nuclear many-body problem, where he has developed and deployed the innovative Auxiliary Field Diffusion Monte Carlo method, which helps unlock insights into nuclei and dense neutron star matter. Gandolfi's work in LDRD first began in 2011 as a Co-Investigator on a Directed Research project.*

Top 2%

The recognition of individuals as esteemed members of technical staff in an ST&E field is an indicator of career advancement. These staff members are named “Fellows” at LANL, Senior Scientists/Engineers at Sandia National Laboratory, and Distinguished Members of the Technical Staff (DMTS) at Lawrence Livermore National Laboratory. The shorthand name used here, “Top 2%,” comes from the intent at each of these Laboratories to limit membership to the top 1% or 2% of scientific and technical staff. The Top 2% awards are comparable to a lifetime achievement award, in this case, for contribution to the Laboratory’s mission.

In FY24, all seven of the LANL staff awarded the Fellow recognition had prior experience with LDRD. Fellows typically gain LDRD experience early in their careers, with an average of about 14 years from their first LDRD experience to being named a Fellow.

LDRD and Top 2% Fellows at Los Alamos National Laboratory

	Single-Year Statistics			Five Years		Ten Years
	FY22	FY23	FY24	FY15-FY19	FY20-FY24	FY15-FY24
Total Awards	9	9	7	24	36	60
Awards with LDRD Roots	9	9	7	20	35	55
% with LDRD Roots	100%	100%	100%	83%	97%	92%
Average Years from First LDRD Experience	17.1	11.6	16.8	14.9	14.1	14.4

Seven LANL Researchers Elected 2024 Fellows have LDRD Experience

***Cynthia Reichhardt**, of the Theoretical division, has had a major impact in both hard and soft theoretical condensed matter physics and in Los Alamos core programs. She is internationally known for her pioneering work on phase transitions in nonequilibrium systems and has produced a prolific output of high-impact journal publications. She is also a fellow of the American Physical Society, served as Chair of the Topical Group on Statistical and Nonlinear Physics, and was awarded a Los Alamos Fellows’ Research Prize. Reichhardt’s work in LDRD first began in 2007 as the PI of an Exploratory Research project.*

***Robert Aikin**, of the Sigma division, has made significant contributions to the field of solidification science and specifically pioneered an integrated experimental and computational approach to applying gravity casting technologies to uranium alloys. His long and productive career has established him as a recognized authority in solidification science and metallurgical processing. Aikin’s work in LDRD first began in 2011 as a Co-Investigator on a Directed Research project.*

(continued on next page)

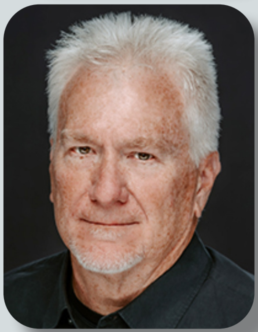
LANL Researchers Elected 2024 Fellows have LDRD Experience

Luis Chacon, of the Theoretical division, has made a series of research contributions that have extended the reach of plasma simulations and defined the state of the art in computational plasma physics. He has deployed his methods to further understand important applications such as magnetic reconnection, inertial electrostatic confinement fusion, inertial confinement fusion and magnetic confinement fusion. Chacon's work in LDRD first began in 2004 as the PI of an Exploratory Research project.

Malcolm Boshier, of the Materials and Physics Applications division, is considered a founder of the field of atomtronics and is a world-leading authority in atomic, molecular and optical physics. Boshier is a recognized international authority on quantum technologies and is regularly sought as a leader on this topic by Laboratory and intelligence community leaders. Boshier's work in LDRD first began in 2003 as the PI of an Exploratory Research project.

Sara Del Valle, of the Analytics, Intelligence and Technology division, revolutionized infectious disease modeling and forecasting by integrating the impact of human behavior into predictive algorithms — an element previously ignored in epidemiological models. This innovation has significantly improved the accuracy and real-world applicability of disease modeling. Additionally, she pioneered the use of novel data streams, such as internet data, enhancing early detection and response efforts in global disease forecasting. Del Valle's work in LDRD first began in 2016 as the PI of an Exploratory Research project.

Rod Linn, of the Earth and Environmental Sciences division, has had a transformative impact on wildland fire science and has made sustained and impactful contributions in weapon effects, wind energy and radioactive waste risk management. His achievements in developing a multi-fidelity suite of coupled wildfire/atmosphere models, including HPC-based research codes and fast-running codes that captured the essential qualities to support prescribed fire practitioners, have led to numerous intergovernmental collaborations. Linn's work in LDRD first began in 2001 as the PI of an Exploratory Research project.



Kevin Mitchell, of the Chemistry division, has more than 20 years of experience in remote sensing, specializing in spectral data analysis. From 2012 to 2018, he led the Remote Sensing team in the Chemistry division, building a team known for delivering comprehensive research solutions related to global security issues. Currently, he serves as a senior scientist overseeing remote sensing projects and is recognized for his technical leadership in tradecraft development for the Department of Energy and partner agencies. His current research focuses on applying machine learning to spectral imaging. Mitchell's work in LDRD first began in 2008 as the Co-Investigator of a Directed Research project.

Workforce Development

American Chemical Society Fellow

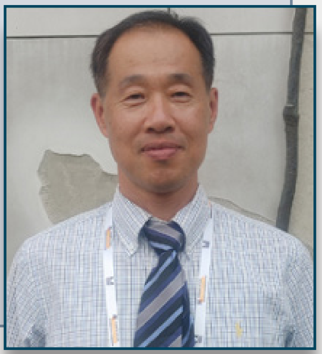
***Jennifer Hollingsworth** of the Center for Integrated Nanotechnologies in the Lab's Materials Physics and Applications division has been selected as a fellow of the American Chemical Society. Hollingsworth's recognition stems from her nanomaterials work with quantum dots, her mentorship and leadership within the chemistry community and her service to the society.*

Hollingsworth's research has played a pivotal role in the discovery and development of nonblinking giant quantum dots, understanding and controlling the fluctuation of single quantum dot emission intensity. With pioneering contributions to materials chemistry, nanomaterials photophysics and optoelectronics applications, Hollingsworth is the author of numerous impactful publications over her 25-year career. She has served as the leader of the Nanophotonics and Optical Nanomaterials thrust at CINT since 2018.

Hollingsworth joined the Lab in 1999 as a director's postdoctoral fellow. She was named a Laboratory Fellow in 2016. In 2018, she was honored as a fellow of the American Physical Society, Division of Materials Physics, and in 2019 as a fellow of the American Association for the Advancement of Science, Chemistry, Section C. She received her doctoral degree in inorganic chemistry from Washington University in St. Louis in 1999 and her bachelor's degree in chemistry from Grinnell College in 1992, Phi Beta Kappa.

Additional LDRD Spotlights

Workforce Development



LDRD Researcher receives Electrochemical Society Award for Sustainable Energy Technology

Laboratory materials scientist Yu Seung Kim has been honored by the Electrochemical Society (ECS) for his significant contributions to fuel-cell innovation. Kim received the Energy Technology Division Walter van Schalkwijk Award in Sustainable Energy Technology. His research, validated through both theoretical and experimental studies, has advanced the performance of high-temperature proton exchange membrane (HT-PEM) fuel cells.

Kim's advancements in HT-PEM fuel cells allow the cells to operate efficiently at elevated temperatures, removing the need for bulky radiators and air intakes. His team's development of polymer electrolytes allows enhancing fuel cells' power density by 60% while showing minimal degradation over conventional HT-PEM fuel cells.

Kim joined Los Alamos National Laboratory in 2003 following a postdoctoral fellowship at Virginia Tech. Kim earned his doctoral degree in chemical engineering from the Korea Advanced Institute of Science and Technology and his bachelor's degree from Korea University. Kim's work with LDRD first started in 2016 as a Co-PI on an Exploratory Research project focused on flow cells for energy conversion and storage.

LDRD Researcher receives DOE Hydrogen Program Lifetime Achievement Award

The DOE Hydrogen Program has recognized Laboratory materials scientist Piotr Zelenay with a lifetime achievement award for his outstanding contributions to the fields of electrocatalysis and electrochemistry.

Zelenay's research focuses primarily on fundamental and applied aspects of polymer electrolyte fuel cell science and technology, electrocatalysis and electrode kinetics. A LANL, Electrochemical Society, and International Society of Electrochemistry fellow, Zelenay joined the Los Alamos Fuel Cell Program in 1997. During his more than 45-year career, he has held teaching and research positions in universities throughout Europe and the U.S.

Zelenay holds Ph.D. and D.Sc (habilitation) degrees in chemistry from the University of Warsaw, Poland, as well as a National Professorship in Chemistry, which was awarded by the president of Poland in 2015. Zelenay's LDRD work first began in 2007 as PI on an LDRD Exploratory Research project focused on fuel cell catalysis research.

R&D 100 Awards

Technical Vitality

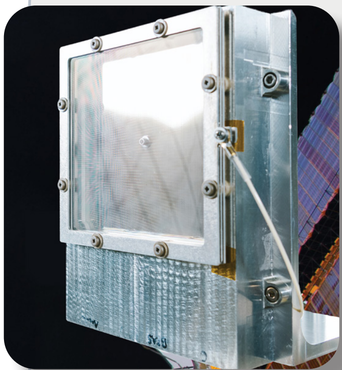
A relevant indicator of advancement and leadership in an ST&E field is the R&D 100 Award. The prestigious "Oscars of Invention" honor the latest and best innovations and identify the top technology products of the past year. The LDRD Program Offices at each site often partner with sister organizations, such as the Intellectual Property Office and Public Affairs, to track whether R&D 100 winners (whether in the standard category or special awards) have "LDRD roots." Because of the long development time from idea to practical implementation, the staff on an R&D 100 Award may not be the same staff who worked on the original R&D. Each site's LDRD Program Office engages in an extensive interview process to uncover the details of how the LDRD work led to the celebrated invention.

In FY24, six of the eight R&D 100 Awards received by LANL have roots in LDRD. While there is sometimes minor fluctuation from year to year, multi-year analyses consistently reflect a majority of R&D 100 winners with prior LDRD experience. Of the 73 R&D 100 awards received by LANL since FY15, 45 have roots in LDRD.

LDRD and R&D 100 Awards Earned by Los Alamos National Laboratory

	Single-Year Statistics			Five Years		Ten Years
	FY22	FY23	FY24	FY15-FY19	FY20-FY24	FY15-FY24
Total Awards	9	9	8	32	41	73
Awards with LDRD Roots	6	5	6	18	27	45
% with LDRD Roots	67%	56%	75%	56%	66%	62%
Average Years from First LDRD Experience	9.3	4.8	3.5			

In 2024 Los Alamos led eight R&D 100 winners. Six of the awards have roots in LDRD. The following awards are those with LDRD roots.

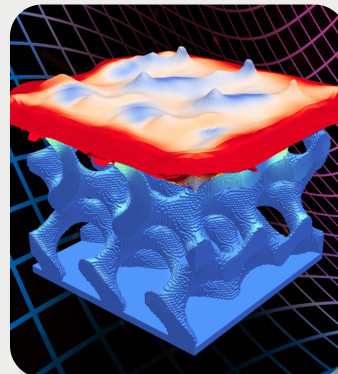


Compact Space Plasma Analyzer

The space plasma environment can damage satellites and interfere with communication signals. Researchers have developed the low size, weight, and power sensor to monitor satellite environments and protect assets for commerce and national security applications. Three years after initial concept, the Department of Defense Space Test Program deployed the analyzer on the International Space Station for data collection.

Los Alamos led the joint entry with the United States Air Force Academy. Carlos Maldonado directed the Los Alamos team of Daniel Reisenfeld, Kateryna Yakymenko, Gabriel Wilson, Justin McGlown, Anthony Rogers and Tatiana Espinoza. Watch the video.

Fierro Computational Mechanics and Materials Science Software



To advance engineering and manufacturing applications, multiscale physics solvers predict product behavior by modeling how detailed material properties and microstructure influence bulk-scale performance under various conditions. Advanced artificial intelligence techniques that search for the optimal design among millions of design options, combined with the flexibility of additive manufacturing to create parts, paves the way for transformative improvements to engineered systems. The combination of numerical methods, models and computer science leads to enhanced products and cost savings across a wide range of industries and applications.

Nathaniel Morgan led the Los Alamos team with Ricardo Lebensohn. The team members are Vincent Chiravalle, Adrian Diaz, Daniel Dunning, Erin Heilman, Sarah Brown, Evan Lieberman, Konstantin Lipnikov, Mounia Malki, Russel Marki, Lorenzo Micalizzi, Jacob Moore, Andrew Morgan, Eappen Nelluvelil, Robert Robey, Calvin Roth, Tayna Tafolla, Svetlana Tokareva, Joshua Vedral, Steven Walton, Kevin Welsh, Caleb Yenusah and Miroslav Zecevic. Watch the Video.

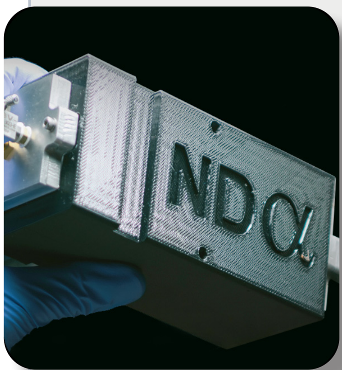
MENDS (Modular Electrochemical Nuclear Decontamination System)

The self-contained, scalable system removes radioactive contaminants on surfaces that impact nuclear industries, such as nuclear energy, national laboratories and nuclear medicine. The technology uses a fixed volume of internally generated and recycled solution to decontaminate surfaces to safe, low-level waste limits. MENDS promotes worker safety, eliminates the need for intensive manual labor leading to ergonomic injuries, and reduces generation of secondary waste. MENDS is poised to advance green methods for recycling and recovery of rare earth metals, mitigating biofouling and enhancing adherence of protective coatings.

Rami Batrice led the Los Alamos team of Cesar Dominguez, Janelle Droessler, Benjamin Karmiol, Sean Walsh, Gabriel Andrade, Sheldon Apgar, Jerzy Chlistunoff, Enkeleda Dervishi-Whetham, Alp Findikoglu, George Goff, Tye Jorgenson, Taeho Ju, Alexandria Marchi, Quinn McCulloch, Jackson McFall, Marisa Monreal, Jeremy Monroe, Donivan Porterfield, Jung Rim, David Rodriguez, Kirk Weisbrod, Bryan Steinfeld, Jared Stritzinger and Ning Xu.

MENDS also received the Gold Medal Special Recognition Award for Green Tech, which honors innovations that help make our environment greener and our goal towards energy reduction closer. Watch the video.

(continued on next page)



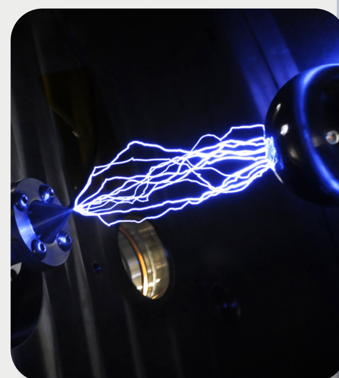
NDa (Nondestructive Alpha Spectrometer)

Alpha radiation measurements of plutonium, uranium and other actinides require time-consuming destructive sample analysis in a special laboratory. Researchers have created the first field-deployable alpha spectrometer for surface scanning of material noninvasively, quickly and safely. Such measurements are needed after a nuclear incident, as well as applications in nuclear power, environmental remediation and targeted alpha therapy in nuclear medicine.

Mark Croce and Katherine Schreiber led the Los Alamos team of Matthew Carpenter, Daniel McNeel, David Mercer, Emily Teti, Rico Schoenemann, Athena Marenco, Hye-Young Lee and Istvan Robel.

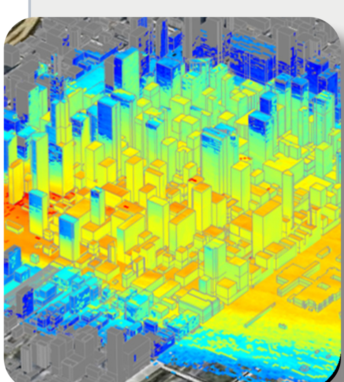
NDAlpha also received the Silver Medal Special Recognition Award for Market Disruptor, which honors any product or service from any category that has truly changed the game in any industry. Watch the video.

PHOENIX (Portable High-efficiency, Orthovoltage ENergy Imaging X-rays)



To advance This field-deployable x-ray source operates in the orthovoltage (500KV-1MV) energy range, which is significantly more penetrating than medical x-rays. PHOENIX provides high-resolution images in a range of applications previously deemed impractical or impossible for x-ray inspection. The source can be taken to inspect stationary objects, such as bridges and pipelines. PHOENIX eliminates the use of hazardous radioisotopes and portable power generators that other sources require.

The Los Alamos team includes Scott Watson, Nicola Winch, Lauren Misurek, David Platts, Myles Cartelli, Chris Romero and Eric Sorenson. Golden Engineering was a partner on the R&D 100 entry. Watch the video.



QUIC-DEPDOSE: Radiation Aerosol Dispersion and Inhalation Model

Radioactive aerosols can cause radiation doses to workers and the public through inhalation. Los Alamos has developed the software to calculate radiation doses from inhalation of radionuclides downstream from an atmospheric radiological release. QUIC-DEPDOSE uses real 3D topography to model the atmospheric dispersion and lung deposition of radiological particles from the scale of kilometers across a city down to microns in the human respiratory tract. Unlike other software, QUIC-DEPDOSE provides accurate, individualized dose information quickly on a laptop to support emergency responders.

Jennifer Harris and Mike Brown were the PI and co-PI, respectively, of the HEROS Project under which QUIC-DEPDOSE was developed. John Klumpp and Matthew Nelson led the Los Alamos team of Luiz Bertelli, Keith Eckerman, Michael Brown, Sara Brambilla and Liam Wedell.

QUIC-DEPDOSE also received the Silver Award for Corporate Social Responsibility, which honors organizational efforts to be a greater corporate member of society. Watch the video.

LDRD Program Accomplishments

Top Science in the News

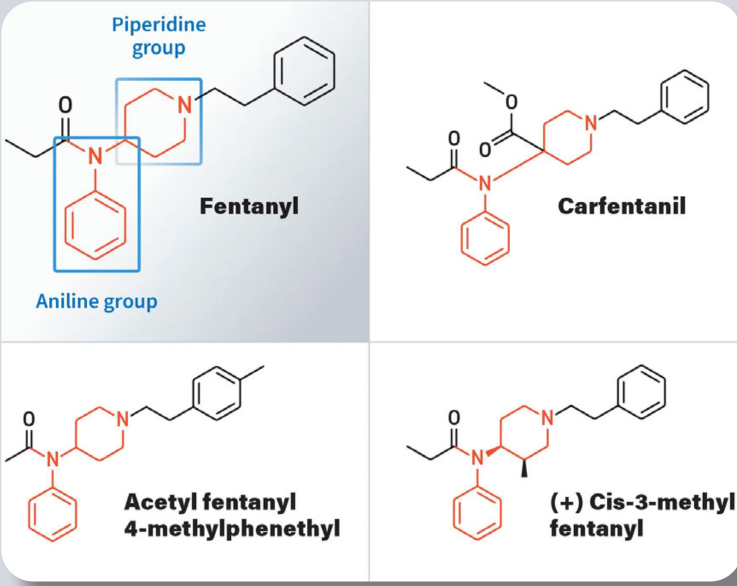
Fighting Fentanyl Overdose

NEW DETECTORS CAN HELP FIGHT THE OPIOID CRISIS BY FINDING DANGEROUS DRUGS AT U.S. PORTS OF ENTRY

Fentanyl is a legal but tightly controlled prescription painkiller. But illicit fentanyl, the knockoff version, is the number one cause of overdose deaths in the United States. It is smuggled into the country by air from Asia and by land from Mexico, hidden in modest packages of otherwise benign contents, like food or toys, and then, once in, it's unleashed into the street-drug market. Catching it at ports of entry is costly and time consuming. Typically, x-ray systems are used to flag anomalies, like hidden compartments in vehicles, then any package that is found and deemed suspicious is opened and the contents analyzed with special spectroscopic or chemical tests. To help break the supply chain of this lethal drug, a Los Alamos team led by researcher Michael Malone is developing an instrument that can screen packages for fentanyl quickly and reliably without even opening them.

The team's approach is centered around two different magnetic resonance techniques, nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR). The fentanyl detector the team is building will use NQR when deployed, but it will be calibrated and validated in the lab by long-standing NMR techniques.

NQR is similar to NMR, but differs in the details. Both techniques use resonant radio-frequency pulses to produce an AC magnetic field from the target nuclei. However, whereas NMR is based on the energy required to reorient small magnetic fields within a larger one, NQR is based on the energy required to reorient small electric charges within a larger electric field. It only works on nuclei with a nonspherical, or quadrupolar, charge distribution, and it only works in an electric field gradient, not a uniform electric field. These constraints mean NQR can only be performed on certain nuclei, namely quadrupolar nuclei, and for certain materials, namely crystalline solids.



There are many different forms of fentanyl. These four fentanyl analogs have slightly different molecular structures, but they all have the same piperidine and aniline groups at their core. Los Alamos scientists are building a detector based on this common core that will catch a broad range of fentanyl analogs.

Each fentanyl analog has a unique NQR frequency, so pinning one down doesn't necessarily lead to the others. "Nitrogen NQR frequencies cover a wide range, and without prior structural or chemical information, they would be impossible to predict," says Harris Mason, a Lab chemist on the team who leads the NMR portion of the project. "Solid-state NMR helps tell the NQR folks where to look. NQR gives nice, sharp, well-defined signal peaks that are perfect for fingerprinting, but you don't know where to find them beforehand, and because they are so narrow, searching by NQR is a pain. It's better to search first using NMR because the peaks are bigger and blobbier and harder to miss."

In other words, the team uses NMR to zero in on the resonant frequencies, then NQR to do the actual detection. One advantage of using NQR for the detector is that the resonant frequencies are chemically unique, making it ideal for chemical detection. Also, NQR is more field-deployable than NMR.

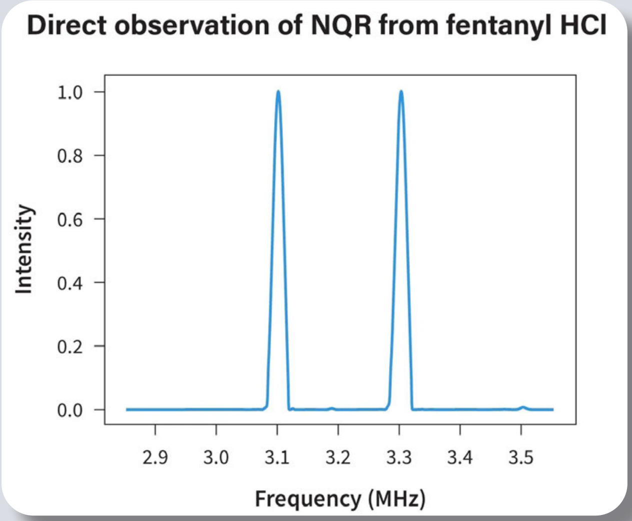
The NQR-based detector system that the Los Alamos team has built currently consists of about 100 thousand dollars of specialized hardware. A powerful radio-frequency amplifier produces the pulses needed to excite the signal, and a specialized spectrometer controls the experiment and processes the data.

The goal, however, is a simplified and portable system consisting of a handheld device, about the size of a clothes iron, containing both the excitation and detection hardware, which is connected to a laptop computer that, along with two digital-analog signal converters, rides in a backpack worn by the user. In addition to being portable, the Los Alamos team want a detector that operates at room temperature and can penetrate simple packaging, seeing straight through cardboard, plastic, glass, and even metallic foils, and it had to do it in under a minute.

In March 2024, after two years of work on the project, the Los Alamos scientists got the first ever NQR reading for any fentanyl analog, using their prototype device on fentanyl HCl.

The successful NQR reading was a big deal because it proved that an NQR-based fentanyl detector is possible, and it also filled a gap in the scientific understanding of these compounds. Now that the scientists have proven that their system works, it's essentially back to the drawing board to examine different analogs, establish limitations, and determine efficacy.

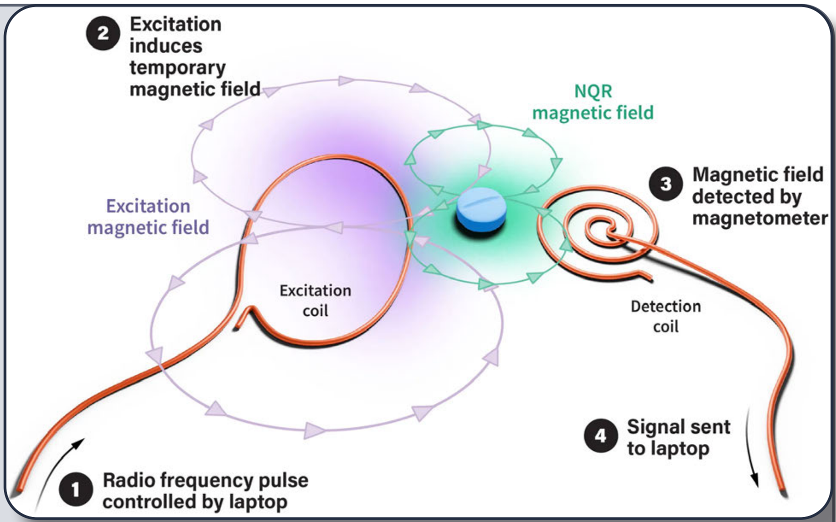
Each NQR signal is a narrow peak somewhere in a very wide spectral space, so unless one knows where to look, it can take a long time to find a signal, and it can be easily missed—like scanning a radio dial for weak or distant channels. The NQR frequencies for fentanyls, the precise frequencies of radio energy that will excite the nitrogen atoms within the molecules, were essentially unknown when the project began, so the Los Alamos team had to start at the very beginning, and the first step was to synthesize their own samples.



The NQR signal produced by the aniline nitrogen atom in fentanyl hydrochloride, a primary illicit fentanyl analog. Distinct narrow peaks are apparent at 3.1 and 3.3 MHz and correspond to the two different possible nuclear orientations of the nitrogen quadrupole. This is the first-ever successful NQR reading from any fentanyl analog.

Some of the necessary physical measurements rely on knowing the crystal structure of the compound, so Laboratory chemist Aaron Tondreau produced a solid crystal of each analog. This allowed Tondreau to determine the compounds' crystal structures via x-ray crystallography, which uses x-ray diffraction to determine the molecular structure of a pure crystalline compound. The method is particularly useful in differentiating closely related materials—like fentanyls—because it provides information about atomic positions, bond types, and bond lengths. These details then get fed back into the computations that predict NQR frequency.

So far, the Los Alamos team has a library of about 25 different fentanyl analogs, representing a variety of salt formulations and chemical modifications. Out of these, the team has solved the crystal structure of about a dozen, including fentanyl HCl—only pharmaceutical fentanyl citrate's crystal structure was previously known. Using this in-house fentanyl library, the team is amassing NMR and NQR data and now has the largest known database of NQR parameters for synthetic opioids.



The portable fentanyl detector that the Los Alamos team will build uses nuclear quadrupole resonance (NQR). The detector consists of a handheld device, about the size of a clothes iron, connected to a laptop in a backpack worn by the user. Although shown here separately for clarity, the excitation and detection coils will be co-located in the handheld unit. The excitation coil produces a pulsed AC magnetic field that drives the nitrogen system in a substance out of thermal equilibrium. After the pulse, the nitrogen atoms return to thermal equilibrium and produce a much smaller AC magnetic field that is observed with the detector coil and quantified by software on the laptop. The result is displayed as either a red light, meaning fentanyl was detected, or a green light, meaning it was not.

NQR signals are not only narrow in frequency, but in time as well. The detector is only looking for the aniline nitrogen, one of the two nitrogens in the fentanyl common core. As the nuclei return to thermal equilibrium, as they relax, the signal dies. You have to be looking at the right place at the right time—blink and you might miss it. To pin down the relaxation properties for the aniline nitrogen in each fentanyl analog, NMR expert Michelle Espy uses fast-field cycling NMR, a technique that uses an externally applied magnetic field, sweeping from low to high, to indirectly observe the NQR system's relaxation rates by interrogating hydrogen nuclei that are coupled to the nitrogen system.

Right now, the detector works like a game of Go Fish: Do you have fentanyl citrate? Do you have fentanyl hydrochloride? Do you have carfentanil? Each analog has a unique NQR frequency and the detector can only ask about one at a time. But the goal is to make it universal, or at least comprehensive. The next generation of detector should be able to interrogate a package about multiple fentanyls at once with a high degree of confidence.

It'll be kind of like the flu shot. Each year, the flu vaccine is designed to target whichever strains of circulating influenza virus are dominant in the population, but it can't possibly cover every strain out there—indeed, it doesn't need to. "It's not realistic to include every single fentanyl analog," explains Malone. "But 50 percent of the market would be great. We could adapt to the analogs that make up the bulk of street fentanyl as it changes over time." So, by calibrating the detectors to the current most likely suspects, the scientists are confident in the coverage they'll achieve.

With their growing library of NMR and NQR data and their increasingly refined mechanical device, the scientists are closing in on the ultimate goal: a practical detector that they hope to demonstrate to authorities within the U.S. Customs and Border Protection, the Department of Homeland Security, and other law enforcement agencies.

The work was funded through LDRD project 20220086DR and led by PI Michael Malone. Read the full article here.

TOP SCIENCE IN THE NEWS

Near-Earth Asteroid Data Helps Probe Possible Fifth Force of the Universe

Bennu and other nearby asteroids. Image Credit: NASA

In 2023, the NASA OSIRIS-REx mission returned a sample of dust and rocks collected on the near-Earth asteroid Bennu. In addition to the information about the universe gleaned from the sample itself, the data generated by OSIRIS-REx might also present an opportunity to probe new physics. As described in the journal Communications Physics, a Nature journal, an international research team led by the Laboratory used the asteroid's tracking data to study the possible existence of a fifth fundamental force of the universe.

Given the implications for planetary defense, near-Earth asteroids are closely tracked. The team applied that ground-based tracking data collected before and during the OSIRIS-REx mission to a probe of extensions of the Standard Model of physics, which describes three of the four known fundamental forces of the universe. Optical and radar astrometric data has helped constrain — or establish to a degree of precision — the trajectory of Bennu since it was discovered in 1999. The OSIRIS-REx mission contributed X-band radiometric and optical navigation tracking data.

The trajectory of a celestial object is impacted by gravity and other factors. Understanding the physics of trajectories can reveal mysteries, especially where there are anomalies in the trajectory. Famously, long before it was actually observed, the planet Neptune was inferred by observations of irregularities in the orbit of nearby planet Uranus.

Using trajectory data and resulting modeling from the tracking of Bennu, the teams' analysis established constraints on a possible fifth force and the role of a potential mediating particle, such as an ultralight boson, in that fifth force. The presence of a mediating particle that might act upon a fifth force would show up in the altered orbit of an asteroid like Bennu, which is why studying the tracking data is so significant for physics.

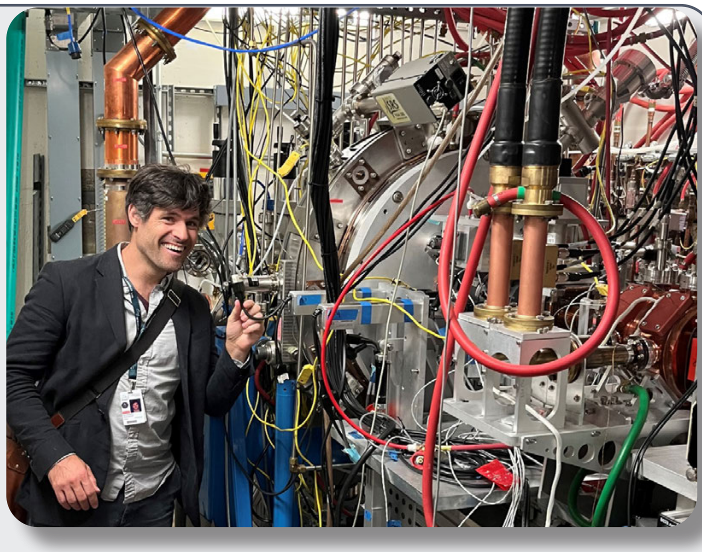
A new particle such as an ultralight boson might represent an extension of the Standard Model to include dark matter and dark energy, which are strongly suggested by cosmological and astrophysical observations but have not yet been incorporated into the general framework. While dark matter is thought to make up perhaps 85% of the total matter in the universe, science remains unsure as to what particles and forces make up dark matter.

The team plans to build on their Bennu work in the future with the tracking of the Apophis asteroid, which will pass within 20,000 miles of Earth in 2029. NASA's OSIRIS-APEX spacecraft will approach the asteroid and kick up dust. That and observations of the impact of Earth's gravity on Apophis as it sails by will provide data to continue the search for fifth-force physics.

This work was supported by an LDRD funded rapid response project in FY22, led by Kai Gao, and by LDRD project 20240477CR, led by PI Chris Carr. Read the article here.

TOP SCIENCE IN THE NEWS

Adjusting accelerators with help from machine learning



LANL physicist Alexander Scheinker develops new ways to use machine learning to improve particle accelerators' performance. Image courtesy of Alexander Scheinker.

Researchers use accelerators to better understand materials and the particles that make them up. Chemists and biologists use them to study ultra-fast processes like photosynthesis. Nuclear and high energy physicists smash together protons and other particles to learn more about the building blocks of our universe. Compact accelerators can be particularly useful for broader applications in society. Medical scientists and doctors use accelerators in cancer therapy, while manufacturers use them to produce semiconductors for electronics. Other applications include sterilizing medical devices, analyzing historical artifacts, and hardening lightweight materials for cars.

Unfortunately, the performance of particle accelerators is prone to drifting over time. They have hundreds of thousands of components. Some of these components are incredibly complex. Influences from outside, like vibrations and temperature changes, can affect how the machinery functions. As various parts shift, they have a domino effect on the pieces after them in line. By the time the accelerator produces the particle beam, tiny shifts may have added up to a significant change. It's like how individual cars slowing down can lead to a traffic jam. Over time, the beam becomes less precise and less useful.

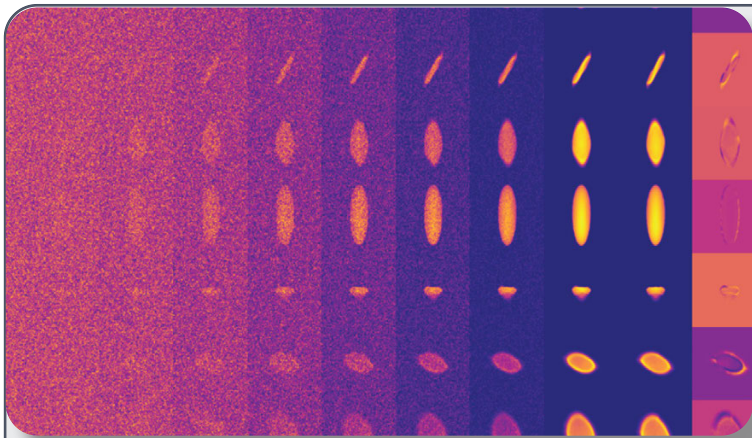
To fix this issue, operators need to "retune" accelerators back to their optimum parameters. These periods of retuning limit how much time the accelerators are available to scientists. In addition, while scientists are taking experimental data, the technicians can't adjust the accelerators in real-time.

On top of all of that, the beams are incredibly complex. They exist in a space that scientists can't measure quickly or even directly. Operators are limited to looking at the beam position in one dimension. Considering that the beam actually exists in six dimensions (the normal three, plus motion in each of them), the operators miss out on a lot of data.

To deal with these issues, scientists have developed complex controls and diagnostics. Special algorithms adapt how a particle accelerator operates to compensate for changes over time. A number of systems use these algorithms. But these methods have a big challenge. Because these algorithms are based on feedback from the accelerator, the algorithms can end up getting "stuck" without finding the true optimal conditions.

Machine learning – a type of artificial intelligence – has the potential to help. With machine learning, computers could act as "virtual observers" that support human technicians.

Machine learning applications are only as good as their training data. Training data are based on the original characteristics of an accelerator. But unfortunately as the accelerator's machinery shifts, those data are no longer accurate! To solve this problem, scientists would have to continuously retrain the model. That defeats the entire point.



A computer-generated image based on a generative diffusion process shows 2D projections of a particle accelerator beam. Starting from pure noise, signals from the accelerator adaptively guide the process. As a result, each version is a little clearer. Image courtesy of Alexander Scheinker.

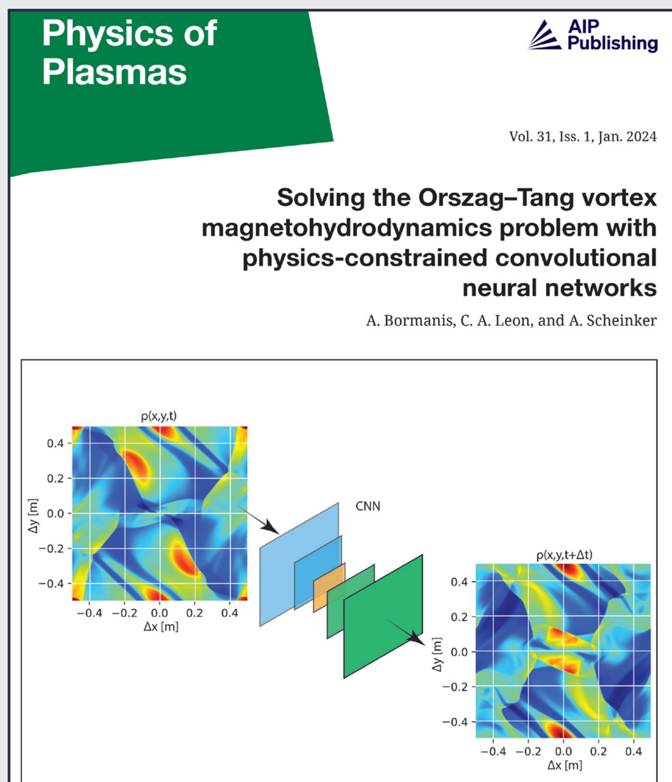
They just end up running into a different variation of their original issue.

The best solution may lie in combining the two approaches. Researchers and engineers at DOE's Los Alamos National Laboratory and Lawrence Berkeley National Laboratory are developing a new machine learning technique for compact particle accelerators. This technique uses real time data from the accelerator diagnostics to continuously tweak the model. It then uses these data to guide an advanced generative artificial intelligence process known as diffusion. The process creates virtual views of accelerators' beams as they change with time. One machine learning tool has the ability to take a set of super complex inputs with many dimensions, compress them into a much simpler representation, and then provide a complex output that reflects the system.

In addition to compact accelerators, these methods can also be applied to large-scale accelerators such as FACET-II. At the FACET-II accelerator system at SLAC (Stanford Linear Accelerator Center), the model produced 15 different two-dimensional projections of the six-dimensional beam at five different locations. While even thinking about that scale hurts a human's brain, the machine learning system needs it. These data allow the system to learn the possible changes over time as well as the changes' relationships with each other and the basic physics. Scientists also demonstrated the adaptability of this approach by showing that the same generative diffusion method can be used at the European X-ray FEL. They used the method to create megapixel-resolution, virtual views of intense electron beams.

So far, this method seems promising. On accelerators where operators can take complex measurements of the beam as it is running, researchers have been collecting data. They then compare the application's predictions to the measurements. With this information, they can further train the application.

The work was supported through the Office of Science's Accelerator R&D and Producation Office and through LDRD project 20220074DR, led by PI Alexander Scheinker. *Read the full article [here](#) and read more about this exciting break through in this recent [cover article](#).*



LDRD LONG-TERM IMPACT STORY

Los Alamos conducts first critical experiment using high assay low enriched uranium in decades

A research team at Los Alamos National Laboratory recently performed the first critical experiment with high-assay low-enriched uranium (HALEU) TRi-structural ISOtropic (TRISO) fuel in four decades at the National Criticality Experiments Research Center (NCERC) in Nevada. It achieved its objective of establishing an advanced reactor testbed.

"With companies such as Amazon and Google investing in nuclear energy to power their data centers, this experiment is extremely important to provide validation data for HALEU," said Holly Trellue, Los Alamos' Engineering Institute leader. "It will help us contribute to the next generation of nuclear reactors in the United States."

As new advanced nuclear reactors are designed and built to use uranium with higher enrichments up to 20%, experiments to understand performance of the material are paramount to designing and licensing new reactor types. Traditional light-water reactors use uranium with enrichment up to 5%.

Through an LDRD project called Next Generation Small Nuclear Reactors, the team conducted an experiment that could improve emerging nuclear technology called advanced and small modular reactors (SMRs), such as microreactors. Microreactors can easily be transported and provide small, mobile power sources. These reactors have numerous applications, including data centers, defense, microgrids, ground operations, oil exploration, providing power to remote villages, and disaster relief.

The experiment used a combination of existing components that have long been in the NCERC inventory, such as the fuel and beryllium reflector, and new components, such as large graphite monoliths containing the fuel. After years of extensive engineering design, components for the experiment were developed and assembled.

The resulting experiment, named Deimos after a Mars moon, required meeting numerous engineering design challenges. Deimos also provides a test bed in which the center portion can be replaced with new materials and geometries relevant to advanced

Members of the Deimos team in front of their experiment in the National Criticality Experiments Research Center.

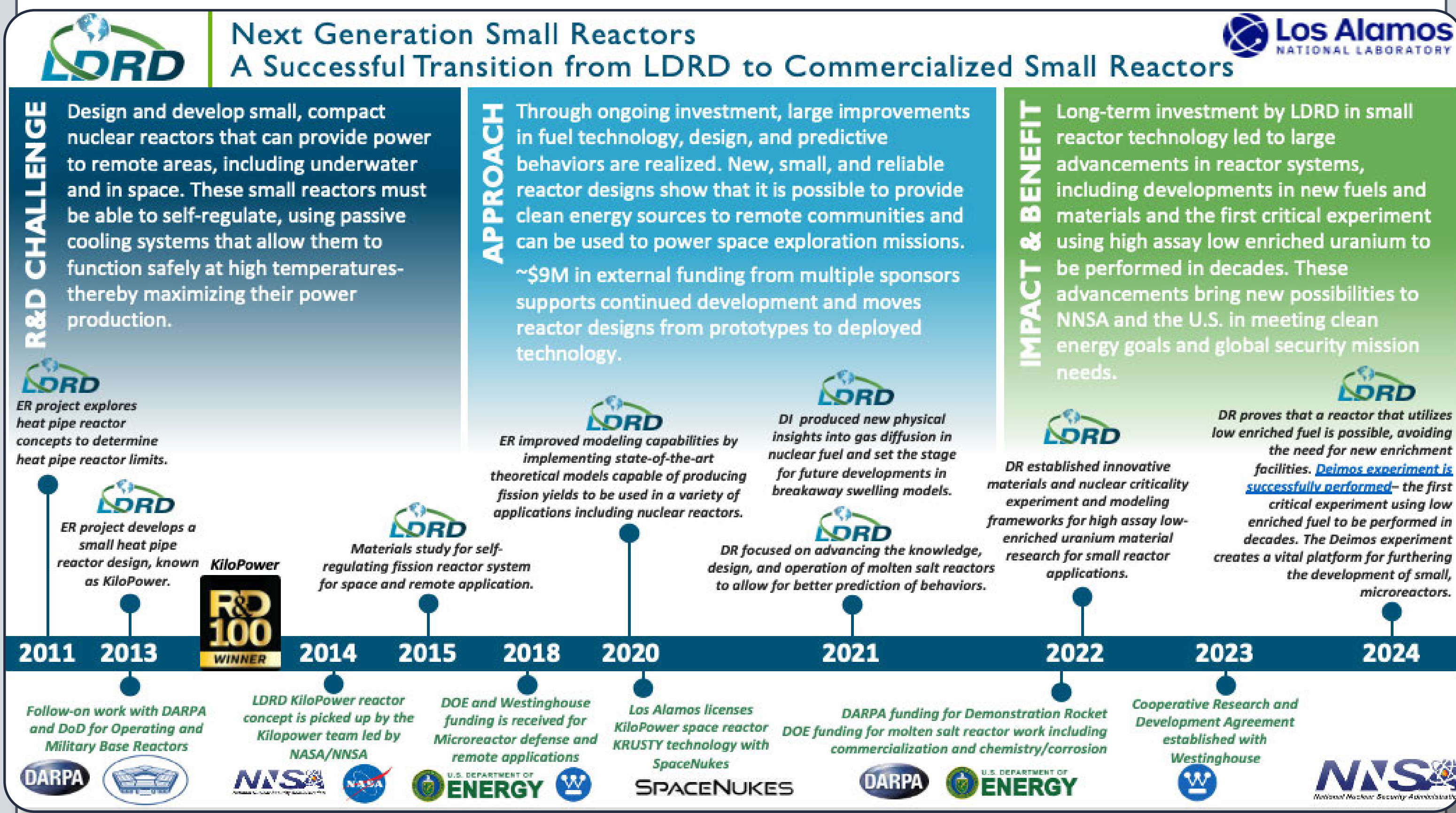
reactor designs driven by HALEU TRISO. Several follow-on projects using Deimos have already been funded.

HALEU TRISO is not a new fuel type. TRISO has been proposed in graphite-based reactor designs for decades and is known to be accident tolerant. A critical experiment called the Compact Nuclear Power Source designed to validate nuclear data and criticality in a graphite-based HALEU TRISO matrix was performed in the 1980s at Los Alamos on a critical assembly machine called Mars, which was decommissioned in 1992.

Resurrecting this capability to perform measurements with TRISO fuel and other materials important to advanced reactors at normal and elevated temperatures is important to supporting validation and verification of simulations before new reactor designs are built.

"Deimos will become a vital platform to further the development of microreactors," said Erik Luther, of Los Alamos' Finishing Manufacturing Science Group and co-lead on the project. "These will be crucial to fulfilling our nation's energy needs."

The work was funded through LDRD project 20220084DR and led by PI Theresa Cutler. Read the full article here.



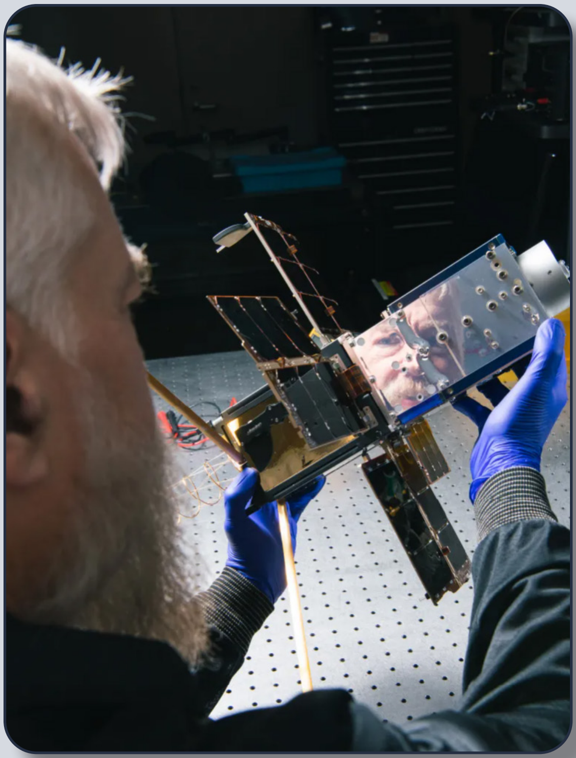
LDRD investments are critical for developing new ideas through innovative research. External investments (in dark green font) are critical for furthering the experimental technology to the point of developing a new capability.

LDRD LONG-TERM IMPACT STORY

Tiny Satellites Big Picture

INSTRUMENTS BUILT INTO SMALL SATELLITES OFFER NEXT GENERATION CHEMICAL ANALYSIS

Thousands of satellites are currently orbiting Earth, serving a variety of uses which include broadcasting, communications, and navigation. Many of these satellites are also used for scientific purposes which can include weather tracking and forecasting, Earth monitoring, and monitoring of atmospheric gases and trace elements that can be used to better understand pollution impact.



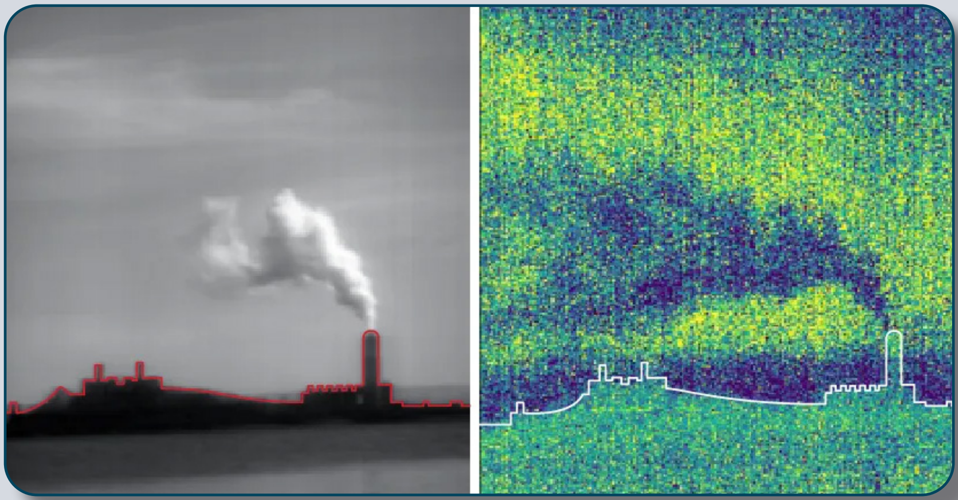
Physicist Steven Love reflects on NACHOS, a CubeSat that was built to carry his team's miniaturized chemical analysis instrumentation.

Most instruments that are robust enough to travel through space and sensitive enough to gather valuable data are large, costly, and require a lot of energy to function. A Los Alamos team led by researcher Steven Love developed an affordable alternative– a small satellite, or CubeSat, called NACHOS (Nano-satellite Atmospheric Chemistry Hyperspectral Observation System) that is the first of its kind. It is a small satellite currently in orbit, purpose-built to "photograph" specific gases in Earth's atmosphere. NACHOS is more than fifty times smaller and lighter than satellites that collect similar data, uses significantly less power, and was designed to deliver high-resolution images. Now, two years into its first deployment, NACHOS is successfully sending home high-quality images of atmospheric gas distributions and demonstrating the possibilities of a whole new era of satellite technology.

NACHOS began its orbit in July of 2022, but its journey to the launchpad began about twenty years ago. Physicist Steven Love, the principal investigator for NACHOS, has spent much of his Los Alamos career developing various types of instruments to detect and study chemicals—often making them smaller to be used for remote sensing. Love, who grew up in Washington state and remembers vividly the 1980 eruption of Mount St. Helens, always had an interest in volcanos and believed remote sensing could be useful for volcano science since many volcanologists make risky trips to get close to eruptions to study their activity. Furthermore, some volcanos are too remote to visit, but their plumes could be of concern when they reach populated areas.

While studying the Popocatépetl volcano near Mexico City—on the ground, a safe distance away—Love's team detected a small but distinct change in the composition of gases just before the volcano erupted, including an increase in SO2 and silicon tetrafluoride. These whiffs of gas piqued the scientists' interest in studying gases that only occur in trace amounts.

Chronic exposure to pollutants such as SO2 and NO2 gases can cause health problems such as asthma, chronic obstructive pulmonary disease, and cardiovascular disease. The World Health Organization estimates that millions of people die prematurely each year due to outdoor air pollution. To thoroughly understand these threats, scientists studying air pollution rely on elaborate data collection stations and direct-sampling point sensors around the world. However, to get detailed data on the atmospheric distribution and chemical evolution of gases such as SO2 and NO2, airborne or space-based monitoring is better because these methods can document the concentration of gases at their points of origin, and then trace how they spread through the air.



NACHOS ground-based images of a power plant near Farmington, New Mexico. (Left) Single-wavelength image from NACHOS. (Right) NO2 matched-filter image produced using NACHOS onboard processing algorithm. High NO2 amounts appear as dark blue and indicate NO2 both in the air as well as pooling near the ground—the latter a key detail missed by other techniques.

Around the time of the Popocatépetl volcano experiments, a technique called hyperspectral imaging was emerging. Hyperspectral imaging is a method that takes a photo of a scene while simultaneously breaking incoming light into its component wavelengths and recording a "picture" of the absorption patterns, so that spectral fingerprints can be used to identify which chemicals are present in the scene and where.

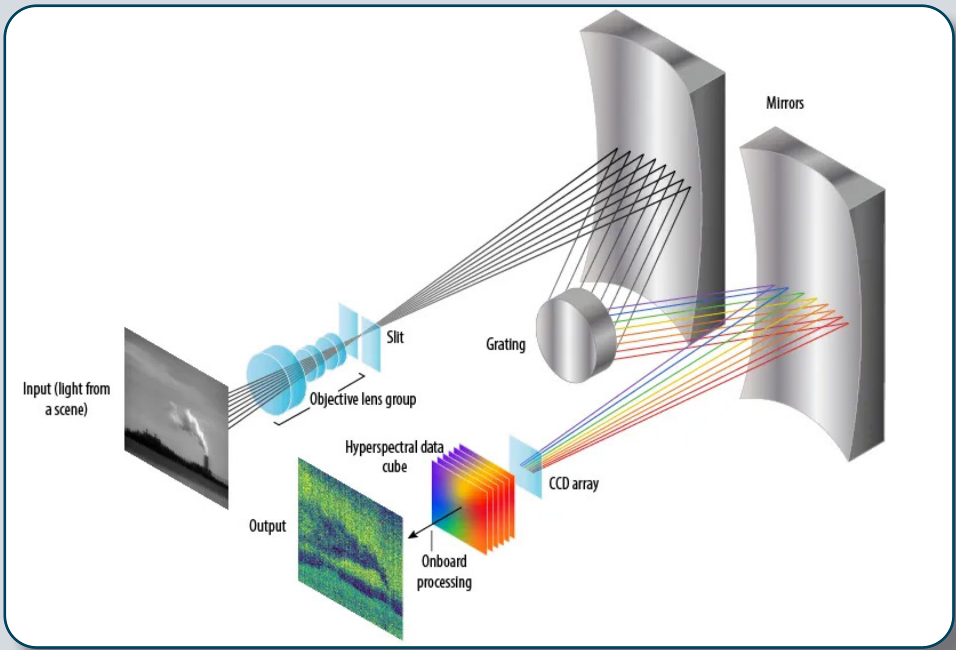
"Hyperspectral imaging is sort of like a super-detailed version of color imaging. It's useful because every pixel of the image contains a high-resolution spectrum with hundreds of wavelength channels—more than just red, green, blue—so you can look at the detailed structure of the spectrum of gases and very reliably distinguish one gas from another," says Love.

As the use of hyperspectral imaging became more widespread, Love recognized its value for detecting trace gases. However, the instruments were massive and required powerful computers that could process very large amounts of data. As a result, many ground-based instruments used hyperspectral imaging, but few satellites had the capability. Love knew if hyperspectral imagers could be smaller and more portable, they could be extremely useful. Love envisioned miniature hyperspectral imagers on drones or even satellites to monitor trace gases—and after years of dedication, he and his colleagues have made it happen.

To fit a hyperspectral imager in a satellite the size of a loaf of bread, Love assembled a team of engineers and software specialists. This project would be a challenge. The team needed to build a small hyperspectral imager but also consider every aspect, from power supplies to the physical robustness needed to survive space travel. The first internally funded project was called Targeted Atmospheric Chemistry Observations from Space (TACOS). The team built an extra-small spectrometer using two concave mirrors and a convex grating component. One mirror directs incoming light to the grating component, which spectrally disperses the light. The second mirror focuses the dispersed light onto a charge-coupled device (CCD) detector array to form the image. Once the TACOS prototype was proven successful, the team received funding from NASA to build it into a CubeSat and launch it into orbit —and the NACHOS project was born.

Since its deployment, the NACHOS CubeSat has been orbiting Earth at an altitude of 500km and will remain in orbit for roughly another year, at which point it will fall back through the atmosphere and burn up. During its time in orbit, the team is working fervently to collect as much data as they can—and they admit there were some challenges at first.

So far, NACHOS has collected data from several sites worldwide, including the Mount Merapi volcano in Indonesia, where it caught the volcano in the act of spewing a plume of ash, and congested cities such as Tokyo and Naples, where it imaged the NO2 smog generated by these cities.

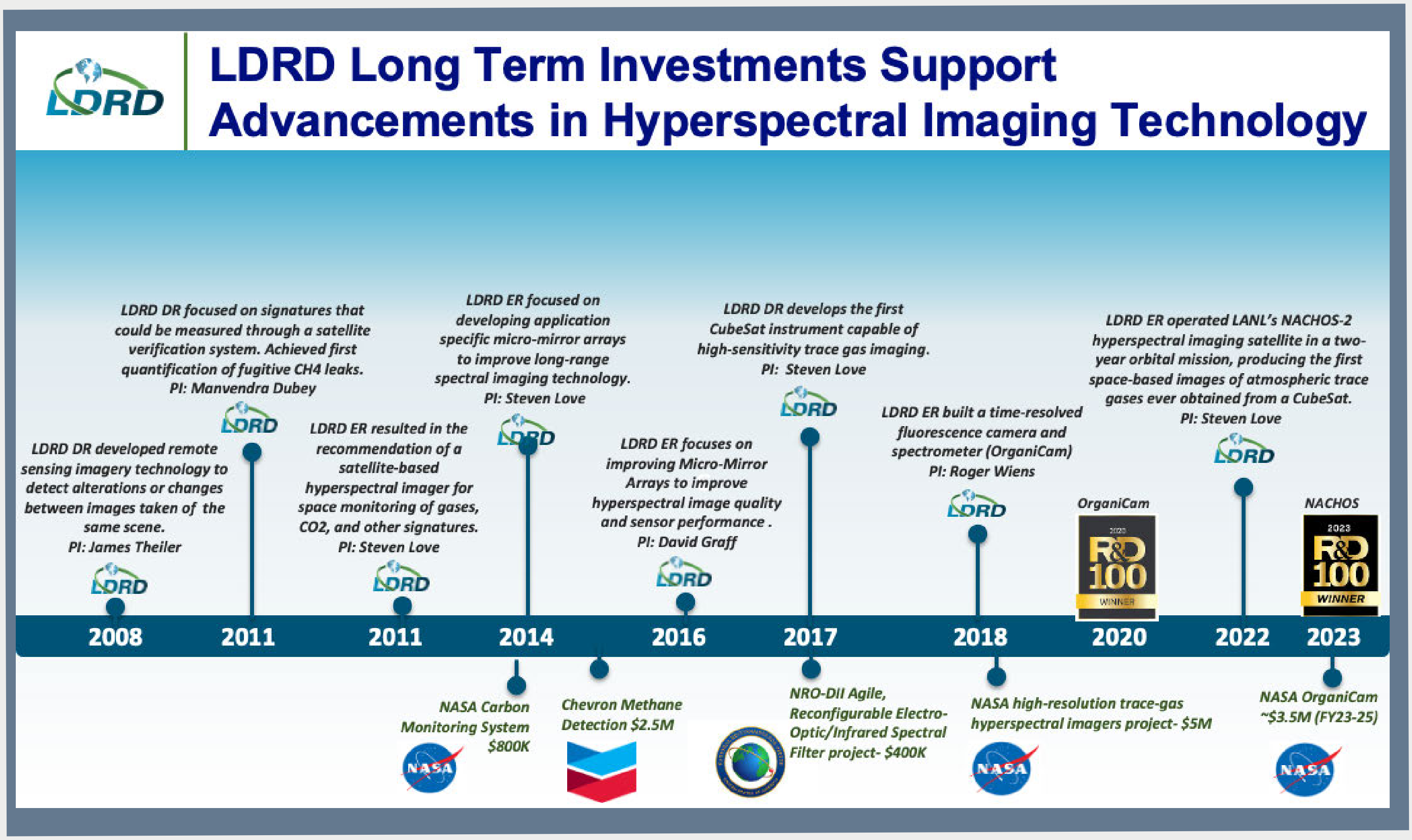


The NACHOS instrument includes a hyperspectral imager, which ordinarily would be a linear series of lenses and prisms, that instead has been folded in half to fit inside the NACHOS CubeSat. Light from a scene enters and passes through a series of lenses and a collimating slit. The light then reflects off a mirror and is directed to a grating component, which spectrally disperses the light. The dispersed light then reflects off another mirror, which directs it onto a charge-coupled device (CCD) detector array to form a data cube of the various spectra. An image can then be constructed using the spectra that correspond to a specific trace gas of interest, showing its concentration and distribution.

Although the clock is ticking on how long NACHOS will be able to collect data before it falls out of orbit, each new target is teaching the Los Alamos team more and more about what their invention can do. Love says that the vision is to one day launch an entire "constellation" of NACHOS CubeSats. With this expanded capability, the team could collect data from multiple targets within a larger geographic area and create a more comprehensive analysis of the distribution and evolution of trace gases. Ultimately, dynamic and agile remote sensing could help lead to better prediction of when a volcano is going to erupt or more detailed smog warnings in city centers.

NACHOS false-color image, taken from low-earth orbit, of central Java, Indonesia, showing the Mount Merapi volcano emitting a plume of ash, and the nearby cities of Semarang and Surakarta.

Read the full article here and watch this video about the NACHOS satellite.



Over a decade of research and investment have gone into developing the hyperspectral imaging technology that is currently onboard the NACHOS CubeSat. LDRD investments were critical for developing the research and proving that the technology could work. External investments (in dark green font) were critical for furthering the technology from a working prototype to a deployed satellite. The image below is a computerized representation of the NACHOS satellite orbiting Earth.

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